NONLINEAR OPTIMIZATION FOR REGIONAL INTEGRATED MANAGEMENT OF GROUNDWATER POLLUTION AND GROUNDWATER WITHDRAWAL

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CERTIFICATE

It is certified that the work contained in the thesis entitled ***NONLINEAR OPTIMIZATION FOR REGIONAL INTEGRATED MANAGEMENT OF GROUNDWATER POLLUTION AND GROUNDWATER WITHDRAWAL*** by ***Ashok Kumar Keshari*** has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

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NONLINEAR OPTIMIZATION FOR REGIONAL INTEGRATED MANAGEMENT OF GROUNDWATER POLLUTION AND GROUNDWATER WITHDRAWAL

An integrated groundwater management model is formulated as a constrained nonlinear optimization problem. The quality and quantity aspects of the groundwater system are conflated in the developed model. To simulate the physical and chemical processes occurring within a leaky confined aquifer system, the coupled set of flow and pollutant transport equations are incorporated into the management model using Embedding Technique (ET). The blended use of quality and quantity aspects into the optimization model avoids the necessity of linking an external simulation model with the optimization model. Thus, the flow and transport processes are simulated within the model. In addition, this model is capable of incorporating other imposed managerial and physical constraints so that the developed optimal policies are operationally, socially, environmentally, economically, financially and politically feasible. This management model is solved using Nonlinear Programming (NLP) because, the embedded solute transport equations are nonlinear. The developed methodology can be used to solve optimization models containing nonlinear constraints and/or nonlinear objectives. Application of NLP also eliminates the necessity of linearizing nonlinear constraints.

Assuming the aquifer as a distributed parameter system, the two-dimensional flow

and solute transport equations are discretized using Finite Difference Method (FDM) in a strong implicit form. These discretized equations are embedded into the optimization model as simulation constraints. The discretized solute transport equation includes the dispersive, diffusive and degradable components in addition to the advective component. However, for illustrative purpose, the applicability of the developed methodology has been demonstrated for cases in which convective diffusion predominates over molecular diffusion. Three types of boundary conditions namely, Dirichlet type, Neumann type and Cauchy type are considered for illustrating the performance of the model.

The developed multivariable constrained nonlinear optimization models are converted to multivariable unconstrained nonlinear optimization models using the Exterior Penalty Function Method (EPFM). The method is chosen over Interior Penalty Function Method (IPFM) to avoid the necessity of specifying an initial feasible solution. The EPFM is also preferred over the IPFM to eliminate some other computational difficulties especially associated with nonlinear equality constraints. The sequential unconstrained minimizations of the resulting composite objective functions are carried out using two different pattern search methods namely, Hooke-Jeeves (HJ) method, and Powell's Conjugate Direction (PCD) method. The PCD method employs the Quadratic interpolation technique (QFIT) for one dimensional search which uses Equal Interval Search Technique (EIST) for bracketing the optimum in one dimensional search. These two methods are preferred over gradient based methods mainly because, evaluations of derivatives are not required and many other computational difficulties are eliminated.

The applicability and suitability of these two methods (HJ and PCD) are explored in terms of their robustness, versatility, accuracy, efficiency and computational

feasibility. The necessary modifications required in the implementation of the IIJ and PCD algorithms for solution of various groundwater management problems are devised and incorporated in the methodology presented. Nonlinear test problems are solved using the developed algorithms and then compared with the exact solutions to validate the coded algorithms. The performance of the developed integrated management model is also tested extensively for descriptive evaluation.

The applicability of the model is illustrated for four distinct types of groundwater management problems. These problems are: (i) Integrated management for groundwater supply, (ii) Integrated management for groundwater remediation, (iii) Radionuclide pollutant management, and (iv) Special case of quantity management. The first and second categories of problems deal with a conservative pollutant, chloride. The third problem deals with a radioactive pollutant, tritium. The fourth problem deals with a groundwater extraction problem in which either quality aspect is irrelevant or ignored. Basically, all these problems are solved by two models: the first one maximizes the objective function and the second one minimizes the objective function.

The first model (Model I) is applicable for the first, third and fourth problems. Model I aims at finding the optimal pumping policies for maximizing the groundwater withdrawal from the aquifer in a planning horizon subject to imposed physical and managerial constraints. The second model (Model II) is applicable for the second problem. Model II aims at finding the optimal pumping policies for minimizing the groundwater withdrawal from the aquifer in a planning horizon, to restore the aquifer upto desired quality under specified operational conditions. The problems are solved to assess the significance of adequately modeling the system and to evolve optimal policies

for different aquifer environment and operating conditions. The solutions are obtained for different management scenarios representing different boundary conditions, aquifer parameter estimates, physical and managerial constraints, and natural as well as man-made processes affecting the groundwater system.

A comparative study of HJ and PCD methods is carried out to assess the applicability and suitability of these two methods for the solution of various groundwater management problems. These comparisons are made in terms of accuracy, efficiency, robustness, ease in implementation and computational feasibility. Solutions for different management scenarios are obtained using both the methods in conjunction with exterior penalty function method and these solutions are then compared. In addition, the computational difficulties encountered during the development of the methodologies and the remedial measures adopted are discussed with proper explanation.

The proposed integrated management model (Model II) is extended to a multiobjective management model in order to evolve policies when conflicting objectives are involved. The formulation, development and solution of the multiobjective management model with two conflicting objectives are illustrated. Solutions of this model provide an optimal management strategy to control pollution distribution in the aquifer as per agricultural needs and at the same time evolve an optimal allocation policy to satisfy irrigation demands. Pareto-optimal solutions representing the tradeoff between the two noncomensurate objectives are obtained using the Constraint Method (CM). The two conflicting objectives considered are: (i) minimization of pumping requirements, and (ii) minimizing the maximum concentration of a pollutant in the aquifer. Physical constraints representing the flow and transport processes, boundary conditions and other

required physical, managerial and operational constraints are also imposed.

The general conclusions of this study are enumerated below:

1. The developed methodologies can be used for regional scale management of groundwater systems.

2. The embedded optimization model is suitable for optimal management of groundwater pollution and groundwater withdrawal. The embedding technique eliminates the requirement of linking flow and transport simulation model to the optimization model externally.

3. The blended use of the flow and solute transport model equations as simulation constraints in the developed integrated management model enables the decision makers to evolve management policies for optimal use of groundwater and its sustainable development in terms of both quantity and quality.

4. The developed methodologies can be used to solve optimization models containing nonlinear constraints and/or nonlinear objectives. Application of NLP also eliminates the necessity of linearizing nonlinear constraints.

5. The Hooke-Jeeves method in conjunction with exterior penalty function method (EPFM & HJ) appears more robust and versatile in its applicability and suitability to solve various groundwater management problems. However, in some situations the Powell conjugate directtion method in conjunction with exterior penalty function method (EPFM & PCD) may prove to be more efficient in locating the optimal solution.

6. Rate of convergence of EPFM & PCD is more than EPFM & HJ, but the former requires more CPU time and computer memory storage.

7. The solution results obtained are dependent on specified initial solution, penalty parameter values and optimization parameters. In no case, a global optimal can be guaranteed.

8. The spatial and temporal distributions of optimal pumping are very much dependent on the specified boundary conditions, initial conditions, aquifer parameter estimates, natural and man-made processes affecting the system, and imposed physical, managerial, operational and other constraints.

9. The proposed model can be easily extended to a multiobjective model to incorporate multiple objectives.

10. The exterior penalty function method together with the embedding approach can be a powerful tool for large scale management of groundwater resources.

11. The applicability of the developed methodologies to solve a problem of large dimensionality will depend on the computing power available. However, computational difficulties associated with scaling, sparse matrices and infeasibility of the solutions are not encountered frequently.

12. Simple modifications of the models are required to incorporate various objective functions, other constraints and complex boundary conditions suitable for different real-life situations.

TO

MY LATE BELOVED MOTHER

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December, 1994 **Ashok K. Keshari**

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NOTATION

a, b, g, h	coefficients of components A, B, G and H in a stoichiometric equation respectively
a_{ijkm}	dispersivity of the aquifer
a_o, a_1, a_2	coefficients to express one dimensional nonlinear function as a quadratic function
a_{xx}, x_{xy}, a_{yx}, a_{yy}	exponential aquifer parameters to define hydraulic conductivity
A	cross-sectional area
[A], [B]	molar concentration of reactants A and B respectively
A_c	area under crop
A_d	area for which nonagricultural water demand is needed
B	boundary of aquifer domain
B	base period of crop
B_{syst}	extensive property of the system
b	thickness of confined aquifer
C	concentration of pollutant
$\underline{C}$	class vector for concentration variables
CS	control surface
CV	control volume
C_l	solute concentration in leakage
C_{lb}	lower bound on concentration variable
C_r	solute concentration in recharge
C_r	Courant number

C_{rx}, C_{ry}	components of Courant number in x and y-directions respectively
C_u	consumptive use of water by crop
C_{ub}	upper bound on concentration variable
d	representative microscopic length characterizing the solid matrix
dA	differential area
dx, dy	differential length of control volume in x and y-directions respectively
$d\upsilon$	differential volume
D	coefficient of mechanical dispersion
D_d	coefficient of molecular diffusion of the solute in the liquid phase
D_d^*	coefficient of molecular diffusion in a porous medium
D_{ij}	mechanical dispersion tensor
$(D_d)_{ij}$	molecular diffusion tensor
$(D_h)_{ij}$	hydrodynamic dispersion tensor
D_L	longitudinal dispersion coefficient
D_T	transverse dispersion coefficient
D_{xx}, D_{yy}, D_{xy}, D_{yx}	components of mechanical dispersion coefficient in two dimension
D_{hxx}, D_{hyy}, D_{hxy}, D_{hyx}	components of hydrodynamic dispersion in two dimension
e	direction vector matrix
e^i	i^{th} linearly independent direction vector
e_{mag}	magnitude of direction vector e^{n+1}

$[e]_{initial}$	direction vector matrix at beginning of search
$[e]_{ng}$	newly generated directional vector matrix
$[e]_{pg}$	previously generated directional vector matrix
$f(.)$	function of given arguments
$f(.)$	original objective function
$f_1(.)$, $f_2(.)$, . . ., $f_6(.)$	function of given arguments
F	mass of pollutant on the solid per unit mass of solid
F	objective function
F_1	objective function for Model I
F_1', F_2', F_3', F_4'	objective functions for different problems
F_2	objective function for Model II
FC	flow coefficients
FC_1, FC_2, . . ., FC_6	components of flow coefficient
$g(.)$	equality constraints
g_f	equality constraint for the flow equation
g_t	equality constraint for the solute transport equation
$g_x(.)$	x^{th} equality constraint
[G], [H]	molar concentration of products G and H respectively
h	hydraulic head
$\underline{h}$	class vector for hydraulic head variables
$h(.)$	inequality constraints

h_s	hydraulic head in source bed
h_{max}	maximum head of water to be lifted
h_{lb}	lower bound on hydraulic head variable
h_{ub}	upper bound on hydraulic head variable
$h_x(.)$	x^{th} inequality constraint
i, j	indices for tensor notation
i,j	indices in positive direction of x and negative direction of y respectively in a finite difference network
I	specified set of grid locations (i,j)
J	hydraulic gradient vector
J_x, J_y, J_z	components of hydraulic gradient vector in x, y and z-directions respectively
k	index for time, t
k'	stage in HJ method
k_b	rate of backward reaction
K_d	distribution coefficient
k_f	rate of forward reaction
K	hydraulic conductivity of an anisotropic medium
K	thermodynamic equilibrium
K_c	hydraulic conductivity class
K_o	order of hydraulic conductivity
K_{xx}, K_{xy}, K_{xz} K_{yx}, K_{yy}, K_{yz} K_{zx}, K_{zy}, K_{zz}	components of hydraulic conductivity
K_{zz}^{ll}	vertical hydraulic conductivity of the leaky layer

l_r	characteristic length ratio
L	characteristic length of the pores
LB	lower bound on decision variable corresponding to ξ_{lb}
L_x	lower bound on the x^{th} objective
m	thickness of the leaky layer
n	outward normal unit vector on control surface
n	normal direction to the boundary
n	total number of decision variables
nc	number of columns in a finite difference network
nr	number of rows in a finite difference network
n_{eff}	effective aquifer porosity
n_p	number of pumps to be installed
nstage	number of stages performed to obtain optimal solution (PCD method)
ntermi	termination parameter to stop execution in PCD method
nts	number of time steps considered within a planning horizon
N	number of atoms at time, t
N_o	number of atoms initially present
p	suffix p refers to pattern move in HJ method
P_e	Peclet number
P_{ex}, P_{ey}	components of Peclet number in x and y-directions respectively
P	pump capacity
$\underline{P}$	class vector for pumping variables
PD	population density
PF_d	peak factor

PF_i	peak factor for irrigation water demand
q	specific discharge vector
$q(.)$	approximated quadratic function of actual nonlinear function
q_x, q_y, q_z	components of specific discharge vector in x, y and z-directions respectively
q_{ca}	advective flux of contaminant
q_{cds}	dispersive flux of contaminant
q_{cdf}	diffusive flux of contaminant
q_{ct}	total flux of contaminant
$(q_{ct})_x$, $(q_{ct})_y$	components of total flux in x and y-directions respectively
q_{cd}	flux of mass of pollutant due to linear rate of decay of pollutant
q_{cad}	flux of mass of linear equilibrium adsorption isotherm of pollutant
q_p	rate of artificial pumping per unit area
q_r	rate of artificial recharge per unit area
q_l	rate of leakage per unit area through leaky layer
q_{pw}, q_{rw}	specific point pumping and recharge from the w^{th} pumping (or recharge) well located at (x_w, y_w) respectively
Q	volume of water flowing per unit time
Q_d	average water supply demand
Q_{lb}	lower bound on pumping variable
Q_{ub}	upper bound on pumping variable
Q_p	pumping
Q_r	recharge
r	set of penalty parameters
R	aquifer domain

R_d	retardation factor
R_e	Reynolds number
R_{ex}, R_{ey}	components of Reynolds number
R_e	effective rainfall in the area during crop period
S	storage coefficient
S_1, S_2, S_3, S_4	specified set of coordinates (x,y) corresponding to the finite difference network
S_5	specified set of cell locations in which pumping is not desired
S_6	specified set of cell locations in which recharge is zero
S_7	set of locations in a finite difference network from which pumping is desired
t	time
tnodv	total number of decision variables
$T_{\frac{1}{2}}$	half-life period of radioactive pollutant
T^*	tortuosity
TC	transport coefficient
TC_1, TC_2, . . ., TC_{10}	components of transport coefficient
$T_{i,j}$	transmissivity tensor
T_{xx}, T_{yy}	principal transmissivities in x and y-directions respectively
U	upper bound on objective function defined by Z_2
UB	upper bound on decision variable corresponding to ξ
v	average velocity through the pores of the porous medium

v_i	average seepage velocity in the direction i
v_k, v_m	velocity components in k and m directions respectively
$\lvert v \rvert$	magnitude of the velocity
v_x, v_y	velocity components in x and y directions respectively
W_l	water required for leaching
W_{kj}	surrogate worth of the tradeoff between the k and j objectives
x, y	coordinate directions
x_i, x_j	cartesian coordinates
x	set of decision variables
x^b	basic decision variable vector
$x^{k'-1}$	previous base point
$x^{k'}$	current base point
$x_p^{k'+1}$	pattern move point
x^o	initial solution vector to start the search process
x^*	optimal solution vector
x_1	any decision variable
x_1, x_2, x	decision variables
$(x_1)_{lb}$	lower bound on decision variable x_1
$(x_1)_p$	decision variable x_1 after pattern move
$(x_1)_{ub}$	upper bound on decision variable x_1
$Z_p(.)$	p^{th} objective function
α, β, γ	radioactive radiations
α	step reduction factor
α_c	reduction factor for concentration variables
α_h	reduction factor for hydraulic head variables

α_q	reduction factor for pumping variables
α_L	longitudinal dispersivity
α_T	transverse dispersivity
β	intensive property of the system
β	acceleration factor
β_c	acceleration factor for concentration variables
β_h	acceleration factor for hydraulic head variables
β_q	acceleration factor for pumping variables
γ	specific weight of water
$\phi(.)$	composite objective function
ϕ_1	composite objective function for Model I
ϕ_2	composite objective function for Model II
$\psi(.)$	objective function which is to be minimized
$\psi(\xi^*)$	optimum functional value in one dimensional search
ψ^b	basic value of objective function
ψ^*	optimal value of ψ
ψ_{io}	inferior solution of the model
ψ_{so}	superior solution of the model
λ	decay constant
ρ	density of fluid
ρ_s	density of soil grains
$\delta(x-x_w, y-y_w)$	Dirac delta function
δ_{ij}	Kronecker delta
δ_p	magnitude of Dirac delta function for specific point pumping
δ_r	magnitude of Dirac delta function for specific point recharge

$(\delta_p)_{i,j}$	magnitude of Dirac delta function for the pumping at node (i,j)
$(\delta_r)_{i,j}$	magnitude of Dirac delta function for the recharge at node (i,j)
$\Omega(.)$	penalty function
Ω_p, Ω_r	index sets of the location of all pumping and recharge cells within the system respectively
Δc	step size for concentration variables
Δh	step size for hydraulic head variables
Δq	step size for pumping variables
Δs	elemental length in flow direction
Δt	time step
Δx, Δy	grid lengths in x and y-directions respectively
Δx^o	perturbation vector
ν	kinematic viscosity
η_a	water application efficiency
η_c	water conveyance efficiency
η_d	water distribution efficiency
η_g	proportion coefficient for groundwater use (agricultural)
η'_g	proportion coefficient for groundwater use (nonagricultural)
η_p	efficiency of pump
ε	termination parameter
ε_{1dv}	convergence parameter for the decision variables in one dimensional optimal search
ε_{1df}	convergence parameter for the function in one dimensional optimal search
ε_c	termination parameter for concentration variables
ε_h	termination parameter for hydraulic head variables

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ε_q	termination parameter for pumping variables
ξ	initial solution for the decision variable in one dimensional optimal search
ξ_1, ξ_2, ξ_3	points in ascending order which bracket the optimum point in one dimensional search
ξ^*	optimum step length in one dimensional search
ξ_c	value of ξ when concentration variables are involved
ξ_h	value of ξ when hydraulic head variables are involved
ξ_n	next value of ξ
ξ_n^*	value of ξ corresponding to the minimum value of nonlinear function
ξ_{opt}	optimal step length in one dimensional search
ξ_p	preceeding value of ξ
ξ_q	value of ξ when pumping variables are involved
ξ_q^*	value of ξ corresponding to the minimum value of approximated quadratic function
ξ_{lb}	value of ξ corresponding to lower bound on decision variable
ξ_{ub}	value of ξ corresponding to upper bound on decision variable
$d\xi$	step size for the decision variable in one dimensional optimal search
$d\xi_c$	value of $d\xi$ when concentration variables are involved
$d\xi_h$	value of $d\xi$ when hydraulic head variables are involved
$d\xi_q$	value of $d\xi$ when pumping variables are involved
x^*	noninferior solution
Ξ	feasible region for the decision variable

INTRODUCTION

CHAPTER 1

INTRODUCTION

Nearly seventy percent of the surface of the earth is mantled in water. Total water available on earth is approximately 1.276 x 10^{18} m^3. Fig. 1.1 shows the distribution of water on earth (Black, 1991). The pictorial representation of this distribution on a broad scale is shown in Fig. 1.1a. The distribution of a relatively smaller quantity of freshwater is shown in Fig. 1.1b. Fig. 1.1c shows the nonuniform distribution of water that is in circulation. However, it should be noted here that some water in each of other three categories shown in Fig. 1.1b are also in circulation. The typical characteristic of water is its dynamic behaviour which constitutes the hydrologic cycle. Water has always been an important factor in the development of a society, as the existence of human life is dependent on the availability of usable water. It is the principal constituent of all living things.

Groundwater constitutes an important component of many water

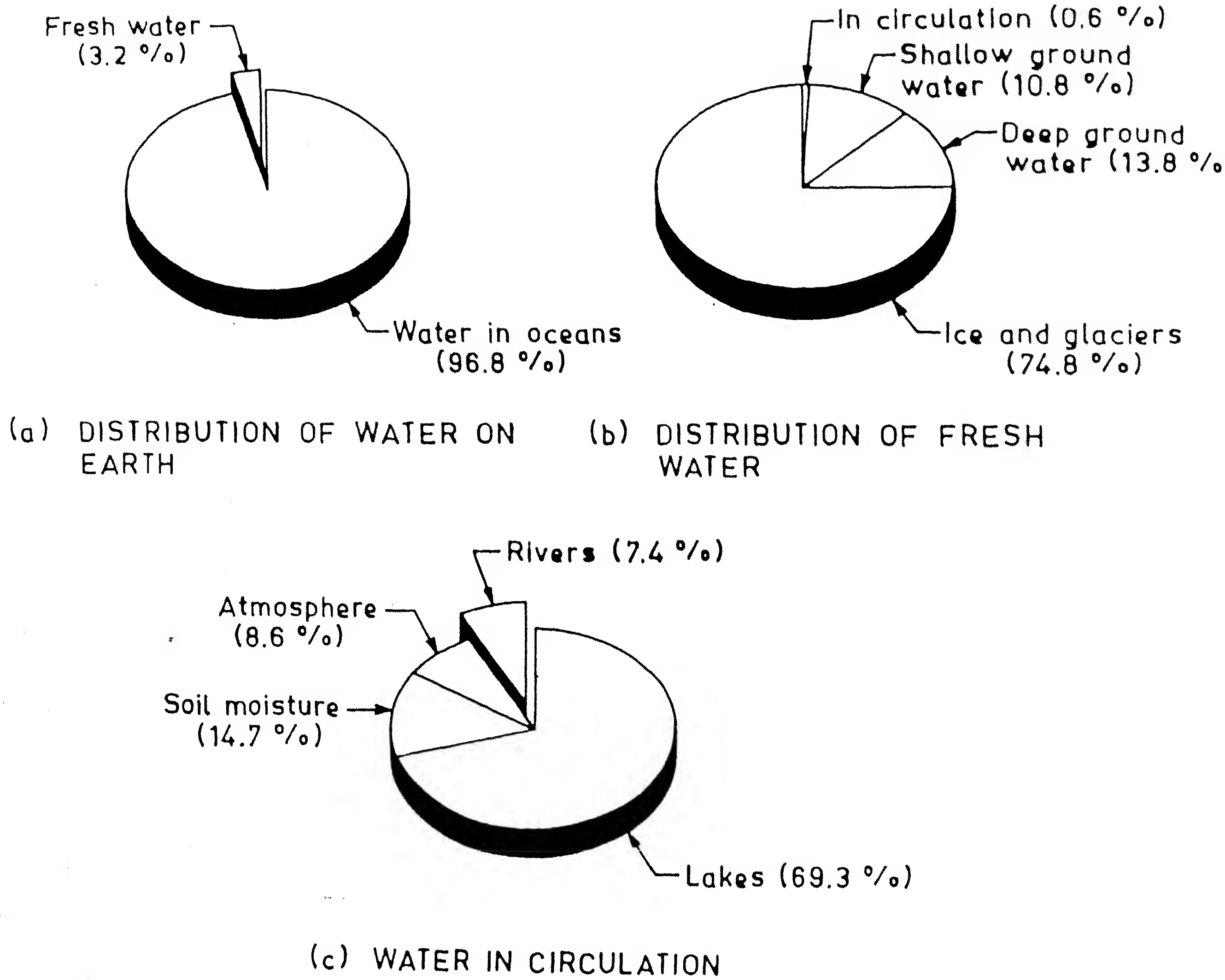


Fig. 1.1. Distribution of water on earth (after Black, 1991)

resources systems that are traditionally developed as sources of municipal, industrial, agricultural and horticultural water supply. Planned withdrawal of groundwater is important particularly in those regions where surface water is nonexistent, inadequate or extremely costly to develop. Again, the quality of surface water as well as groundwater is continuously deteriorating due to rapid industrialization, urbanization and excessive use of agrochemicals for agricultural production. Now a days, deteriorating quality of available water is causing more concern to both suppliers and users of water. Usually the quantity and quality aspects can not be separated and must be treated together. Potential utilization of groundwater not only depends on the availability of water in desired amount, but more crucially depends on its quality that should match the desired or specified quality for various types of uses.

Due to the significance of the quality aspect, management of groundwater systems should not be concerned only with the sustainable development of this natural resource in terms of its quantity alone. Hence, an integrated analysis and management of groundwater pollution and groundwater withdrawal have become essential for both large scale development and smaller scale development or even for an individual well projects. In fact, management of groundwater quality is drawing greater attention within the overall scenario of integrated aquifer management. Therefore, it can be stated that groundwater management involves the planning, implementation and operation necessary to supply reliable

quantities of groundwater having a desirable quality. It involves the formulation and development of the management model to evolve the optimal management policies under different management scenarios. It also involves the analysis of the resulting environmental, hydrologic, political and economic impacts, and derivation of the system tradeoffs associated with the development and allocation of groundwater resources for various purposes.

Mathematically speaking, the integrated management of groundwater quality and quantity of regional aquifer systems can be formulated as a constrained nonlinear optimization problem. The management of a regional groundwater system may have single or multiple objectives depending upon the requirement in specific cases. Depending upon the nature of the flow, groundwater management models can be classified as either nontransient (steady state) management model or transient management model. Containment of groundwater pollution, restoration of aquifers, monitoring of pollutant transport, protection of surface water bodies from contamination by low quality groundwater, management of saltwater intrusion in coastal aquifers, waste disposal activities, conjunctive use of ground and surface waters, as well as parameter identification in regional groundwater basins are examples of some typical groundwater resource management problems.

Mathematical models are indispensable for large scale or regional scale management of groundwater systems. Integrated management models enable the determination of time varying optimal

strategies to meet the desired objective under different management scenarios described by the specified restrictions placed upon hydraulic heads, water supply targets, water quality standards and hydraulic gradients etc. The impacts of implementing a management strategy are obtained as a part of the solution of the optimization model in the form of future time varying spatial distribution of hydraulic heads, water quality and velocity field. These quantities representing the impacts of implementing an optimal management strategy are the numerical values of decision variables associated with the management model.

A management model, a basis for development of an optimal planning or operation strategy is generally a simplified mathematical representation of the real world system with explicitly stated objectives and constraints. It consists of all elements that normally must be considered in describing the physical, chemical and biological phenomena taking place within the system. The formulation of a model is the most crucial step that determines whether the solution obtained by using the developed model will be physically meaningful and realizable. The model should be capable of simulating the excitation response relations of the real world system adequately. Otherwise the outcomes of implementing management decisions will be different from the predicted ones. Simplifying mathematical descriptions of the physical processes and simplifying assumptions for description of the physical system are generally unavoidable in mathematical modeling. Such assumptions also ensure

the computational feasibility of the model. A management model should prescribe optimal planning or operation strategies while adequately modeling the physical processes involved. Management of natural resources like groundwater can be accomplished by the use of an optimization based prescriptive model together with a descriptive model that simulates the flow and transport processes taking place in an aquifer. With the phenomenal increase in computing powers during the last two decades, mathematical models using numerical solution techniques and various optimization algorithms are becoming increasingly feasible and popular. Solution of groundwater resources management problems on a regional scale using such mathematical models is a relatively simple task today.

Once a mathematical model has been constructed in terms of relevant state variables, it is converted into a numerical model by discretization of the governing partial differential equations in space and time. A large sized problem can be handled using numerical models. The numerical model can be solved for simulating and predicting the aquifer response to various applied stresses and contamination histories provided the model has been properly calibrated and validated. In addition, the numerical model may constitute a part of an optimal management model with the discretized governing equations formulated as constraints of the optimization model. These constraints together with the specified objective function and other constraints constitute the optimization model.

The objective of the present study is to develop a methodology for an integrated optimal management of groundwater pollution and groundwater withdrawal. Development of this methodology is motivated by the realization that an optimal management strategy can evolve only when the quantity and quality aspects are integrated in the same decision making process, within a single framework. Solution of such an integrated optimal management model is a challenging task mainly due to the nonlinearities inherent in modeling the flow and particularly the solute transport processes in an aquifer. The explicit objective functions as specified are also nonlinear for many real life management scenarios.

The steps involved in the development of this methodology for solution of such an integrated optimal management model and the performance evaluation of the solution methodology can be categorised as follows:

(i) Formulation of an optimal management model with specified objective functions, physical and managerial constraints, and other embedded nonlinear constraints representing the discretized governing equations for flow and transport processes

(ii) Development of methodologies for solving the resulting multivariable constrained nonlinear optimization model that include two approaches : (a) The Hooke and Jeeves' Pattern Search Method in conjunction with Exterior Penalty Function Method, and (b) the Powell's Conjugate Direction Search Method

in conjunction with Exterior Penalty Function Method

(iii) Performance evaluation of the two methodologies and their comparisons so as to suggest the desirability of a particular approach in solving the integrated management problem.

The integrated groundwater management models presented here consider a single specified objective as well as two-conflicting objectives representing a multiobjective decision model. The Pareto-optimal solutions of the nonlinear two objective decision model are obtained by using the constraint method. Transport of a conservative pollutant (Chloride) and a radionuclide (Tritium) are considered in this study. Optimum management strategies for various management scenarios for different management models are obtained and discussed in detail.

1.1 GROUNDWATER POLLUTANTS AND THEIR SOURCES

The major, secondary, minor and trace constituents that are generally found dissolved in groundwater, and information regarding the range of background concentrations are given in Table 1.1. Table 1.2 lists the radionuclides that are of major interest in groundwater pollution management study. The mass number of radioisotopes and its decay characteristic are also mentioned in this table. In addition to these pollutants, there are natural and synthetic organic compounds which may affect groundwater quality adversely and render the utilization of groundwater for various purposes impossible. Both natural and synthetic organic compounds

Table 1.1 Groundwater pollutants

Major constituents (range of concentration 1.0 to 1000 ppm)

Sodium	(Na)	Bicarbonate	(HCO_3)
Calcium	(Ca)	Sulphate	(SO_4)
Magnasium	(Mg)	Chloride	(Cl)

Silica (SiO)

Secondary constituents (range of concentration 0.01 to 10.0 ppm)

Iron	(Fe)	Carbonate	(CO_3)
Strontium	(Sr)	Nitrate	(NO_3)
Potassium	(K)	Fluoride	(F)

Boron (B)

Minor constituents (range of concentration 0.00001 to 0.1 ppm)

Antimony	(Sb)	Chromium	(Cr)	Lithium	(Li)	Selenium	(Se)
Aluminium	(Al)	Cobalt	(Co)	Manganese	(Mn)	Titanium	(Ti)
Arsenic	(As)	Copper	(Cu)	Molybdenum	(Mo)	Uranium	(U)
Barium	(Ba)	Germanium	(Ge)	Nickel	(Ni)	Vannadium	(V)
Bromide	(Br)	Iodide	(I)	Phosphate	(PO_4)	Zinc	(Zn)
Cadmium	(Cd)	Lead	(Pb)	Rubidium	(Rb)		

Trace constituents (range of consentration generally less 0.001 ppm)

Beryllium	(Be)	Gold	(Au)	Radium	(Ra)	Thorium	(Th)
Bismuth	(Bi)	Indium	(In)	Ruthenium	(Ru)	Tin	(Sn)
Cerium	(Ce)	Lanthanum	(La)	Scandium	(Sc)	Tungsten	(W)
Cesium	(Cs)	Niobium	(Nb)	Silver	(Ag)	Ytterbium	(Yb)
Gallium	(Ga)	Platinum	(Pt)	Thallium	(Tl)	Yttrium	(Y)

Zirconium (Zr)

Source: Davis and DeWiest (1966)

Table 1.2 Radionulides in groundwater

Element	Mass number of radioisotope	Half-life years y days d hours h	Radiation	MPC above natural background μc/ml in solution in water
Barium	131	13 d	γ_-	2×10^{-4}
	140	12.8 d	β_-, γ	3×10^{-5}
Bromine	82	36 h	β_-, γ	3×10^{-4}
Calcium	45	153 d	β_-	9×10^{-6}
Carbon	14	5600 y	β_-	8×10^{-4}
Cerium	144	290 d	β_-, γ	1×10^{-5}
Cesium	135	2.9 x 10 y	β_-	1×10^{-4}
	137	33 y	β_-, γ	2×10^{-5}
Chlorine	56	4 x 10 y	β	2×10^{-5}
Chromium	51	27.8 d	γ_+	8×10^{-3}
Cobalt	57	270 d	β_-, γ	2×10^{-4}
	60	5.3 y	β_-, γ	5×10^{-5}
Hydrogen	3	12.4 y	β_-	3×10^{-3}
Iodine	129	1.72 x 10 y	β_-, γ	4×10^{-7}
	131	8.04 d	β, γ	2×10^{-3}
Phosphorus	32	14.3 d	β	2×10^{-5}
Plutonium	238	92 y	α, γ	5×10^{-6}
	239	2.4 x 10 y	α, γ	5×10^{-6}
	240	6580 y	α	5×10^{-6}
	242	5 x 10 y	α	5×10^{-6}
Radium	226	1620 y	α_-, γ	1×10^{-8}
	228	6.7 y	β	3×10^{-8}
Radon	222	3.83 d	α_-	A gas
Rubidium	86	18.7 d	β_-, γ	7×10^{-5}
	87	6 x 10 y	β_-	1×10^{-4}
Ruthenium	103	40 d	β_-, γ	8×10^{-5}
	106	1 y	β_-	1×10^{-5}
Sodium	22	2.6 y	β_-, γ	4×10^{-5}
Strontium	89	51 d	β_-	1×10^{-5}
	90	29 y	β_-	1×10^{-7}
Sulpher	35	88 d	β	6×10^{-5}
Uranium	235	7.1 x 10 y	α	3×10^{-5}
	238	4.5 x 10 y	α_+, γ	4×10^{-5}
Zinc	65	245 d	β, γ	1×10^{-4}

MPC Maximum permissible concentration

encompass a wide range of substances. Natural organic compounds are classified in three groups depending upon their solubilities in acid and alkali. These groups are (i) humic acid, (ii) fulvic acid and (iii) humins. Synthetic organic compounds include agrochemicals such as fertilizers, herbicides, pesticides; petroleum products such as gasoline, natural gas, kerosene, fuel oils, lubricating oil; surfactants and volatile organic chemicals. The most commonly encountered volatile organic chemicals in groundwater are organohalide solvents and trihalomethanes.

There are two principal sources of groundwater pollution: natural and artificial. Natural pollution occurs as a result of chemical and physical processes that transfer pollution to groundwater from the atmosphere, biosphere or lithosphere. Flow through carbonate rocks; leaching of soluble salts from the soil and rocks; invasion of brackish water, highly mineralized connate water or water associated with volcanic or other special geological formations; seawater intrusion are some of the examples of natural pollution. Overdrafting of coastal freshwater aquifers (a man-made activity) accentuates the seawater intrusion problem.

Waste disposal practices are the most notable human activities affecting groundwater quality. Common artificial sources of groundwater pollution are ponds, ditches and lagoons; stockpiles and wastepiles; industrial wastes; sanitary and nonsanitary landfills; septic tanks, cesspools and privies; irrigation and reclaimed sewage water; and nuclear waste repositories. Other sources include

accidental spills and leaks from underground pipelines, storage tanks and repositories; infiltration from polluted surface waters, canals, mining, oil and gas exploration; agrochemicals used for crop production; animal feedlot wastes; deep well injection of liquid wastes; waste disposal in wet excavations; and drainage wells. Exploratory wells, test holes, and abandoned wells drilled to determine the presence of underground mineral resources such as seismic shot holes also act as sources of groundwater pollution. Groundwater withdrawal activities in some regions or situations may induce significant groundwater quality problems because of interaquifer leakage, induced infiltration, resulting variations in spatial and temporal patterns of pollutant distribution in the aquifer, and induced recharge of surface water towards aquifers. Common commercial operations, such as automotive service, autobody repair, junk yards, dry cleaning, and pinning are often unsuspected contributors to local and regional groundwater pollution. Relevance of these activities in affecting groundwater quality depends upon the local geology, meteorology, and hydrology of the area.

The pictorial representation of these activities is shown in Fig. 1.2. Major pollutants associated with various sources of groundwater pollution are enumerated in Table 1.3 (Roscoe Moss Company, 1990). Detailed discussions on groundwater pollution causes and controls are available in Lehr (1986). The various sources of groundwater contamination are summarized in Table 1.4 (Barcelona et al. 1988).

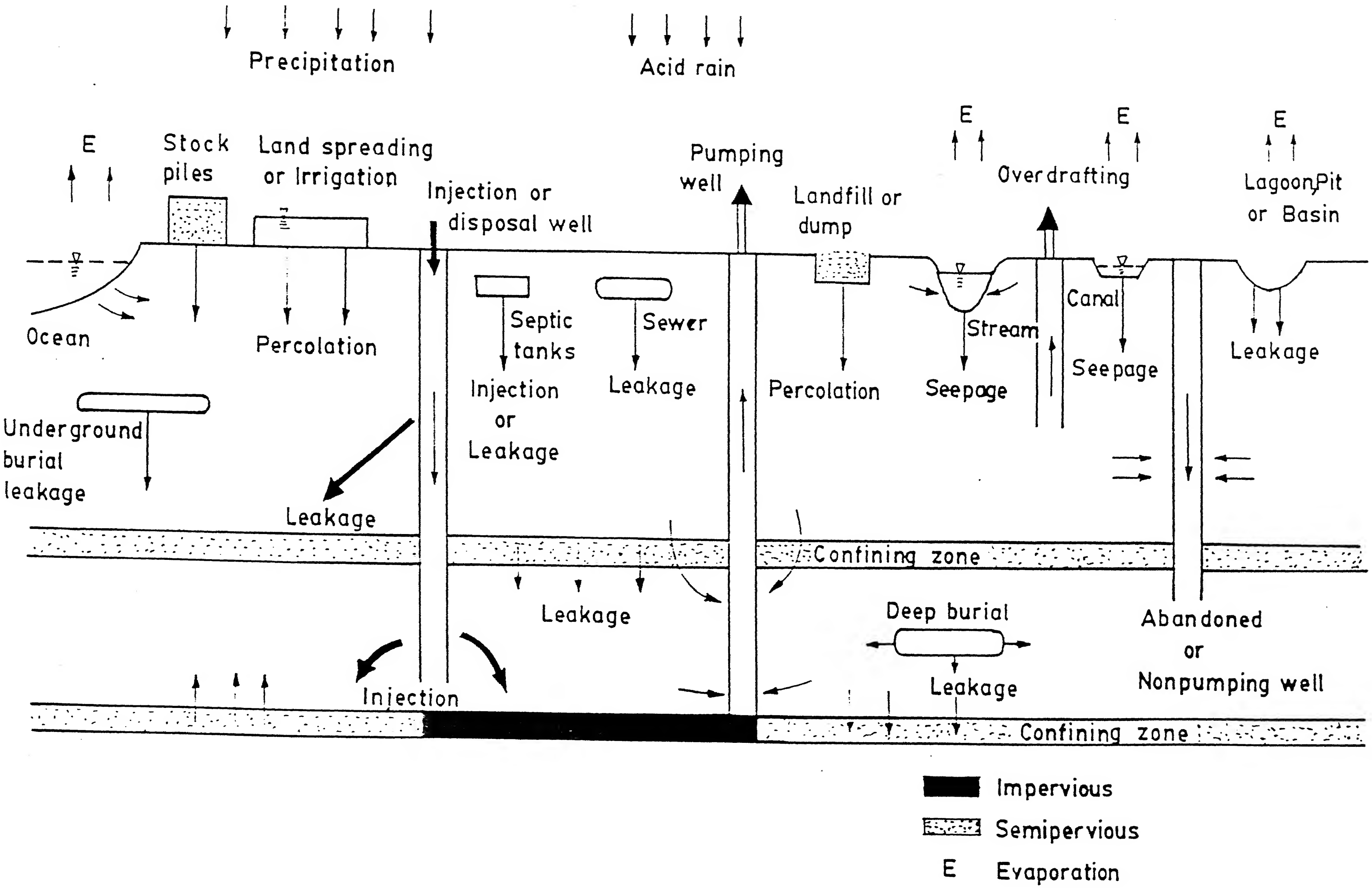


Fig. 1.2 Schematic representation of natural and man-made activities

Table 1.3 Major groundwater pollutants

Source	Possible major contaminants
Landfills	
Municipal	Heavy metals, chlorides, sodium, calcium
Industrial	Wide variety of inorganic and organic constituents
Hazardous waste disposal sites	Wide variety of inorganic (particularly heavy metals) and organic compounds (pesticides, priority pollutants, etc.)
Liquid waste storage ponds (lagoons, leaching ponds, recharge basins)	Heavy metals, solvents, inorganic compounds
Subsurface sewage disposal systems	Organic compounds (degreasers, solvents), nitrogen compounds, sulfates, sodium, microbiological contaminants
Deep-well waste injection	Variety of inorganic and/or organic compounds
Agricultural activities	Fertilizers, herbicides, pesticides
Land application (sludge, waste water)	Heavy metals, inorganic compounds, organic compounds
Urban runoff infiltration	Inorganic compounds, heavy metals, petroleum products
Deicing activities	Chlorides, sodium, calcium
Radioactive wastes	Radioactivity and radionuclides

Source: Roscoe Moss Company (1990)

Table 1.4 Sorces of groundwater contamination

Category I -Sources designed to discharge substance
Injection well
- Hazardous waste
- Non-hazardous waste (e.g., brine disposal and drainage)
- Non waste (e. g., enhanced recovery, artificial recharge, solution mining,and in-situ mining)

Land application
- Wastewater(e.g.spray irrigation)
- Wastewater byproducts (e.g. sludge)
- Hazardous waste
- Non-hazardous waste

Category II - Sources designed to store, treat, and/or dispose of substance; discharge through unplanned release

Landfills
- Industrial hazardous waste
- Industrial non-hazardous waste
- Municiple sanitary

Open dumps,including illegal dumping (waste)
Residential (or local) disposal (waste)
Surface impoundments
- Hazardous waste
- Non-hazardous waste

Waste tailing
Waste piles
- Hazardous waste
- Non-hazardous waste

Material stockpiles (non waste)
Graveyards
Animal burial
Aboveground storage tanks
- Hazardous waste
- Non-hazardous wastes
- Non-waste

Underground storage tanks
- Hazardous waste
- Non-hazardous waste
- Non-waste

Containers
- Hazardous waste
- Non-hazardous waste
- Non-waste

Open burning and detonation sites
Radioactive disposal sites

Category III - Sorces designed retain substance during trans| or transmission
Pipelines
- Hazardous waste
- Non-hazardous waste
- Non-waste

Material transport and transfe operation
- Hazardous waste
- Non-hazardous waste
- Non-waste

Category IV - Sources discharg substances as consequence of o planned activities
Irrigation practice (e.g.retur flow
Pesticide applications
Fertilizer applications
Animal feeding operations
De-icing salts applications
Urban ruhnoff
Percolation of atmospheric pollutants
Mining and mine drainage
Surface mine-related
- Underground mine-related

Category V - Sources providing conduit or inducing discharge through altered flow patterns
Production wells
- Oil (and gas) wells
- Geothermal and heat recovery wells
- Water supply wells

Other Wells (non-waste)
- Monitoring wells
- Exploration wells

Construction excavations

Category VI - Naturally occuring sources whose discharge is created and/or exacerbated by human activity
Groundwater - surface water interactions
Natural leaching
Salt-water intrusion/brackish water upconing (or intrusion and other poor-quality natural water)

Source: Barcelona et.al. (1988)

1.2 MECHANISM OF POLLUTANT MOVEMENT

The processes which govern the transport of a chemical constituent in space and time within a groundwater system are listed in Table 1.5. The present study is concerned with the major processes only. These principal processes are advection (convection), mechanical dispersion (convective dispersion), molecular diffusion, radioactive decay, adsorption, pumping (withdrawal), recharge (injection), and leakage through leaky layer in aquifer system.

The basic transport phenomenon of a pollutant in groundwater is advection. In this mechanism, pollutant is transported due to bulk motion of the fluid in porous media. Dispersion and diffusion cause spreading of the pollutant over an evergrowing region during advection. Dispersion is caused by velocity variations at microscopic level which exist because of the presence of variations in pore sizes, shapes and orientations. Spreading of the pollutant particles are enhanced by molecular diffusion especially in the direction transverse to the average flow. The resulting spreading from both mechanical dispersion and molecular diffusion is called hydrodynamic dispersion. The separation between these two processes is rather artificial. However, molecular diffusion alone also takes place in the absence of motion. The effect of molecular diffusion on overall dispersion is more significant at low velocities. Due to molecular diffusion, hydrodynamic dispersion in purely laminar flow becomes irreversible. Fig. 1.3 shows the spreading of pollutant due

Table 1.5 Processes affecting groundwater pollutant transport process

Physical processes	
	Advection (porous media velocity)
	Hydrodynamic dispersion
	Molecular diffusion
	Density stratification
	Immiscible phase flow
	Fractured media flow
	Pumping
	Recharge
	Leakage
Chemical processes	
	Oxidation-reduction reactions
	Radionuclide decay
	Ion-exchange
	Complexation
	Co-solvation
	Immiscible phase partitioning
	Sorption
Biological processes	
	Microbial population dynamics
	Substrate utilization
	Biotransformation
	Adaption
	Co-metabolism

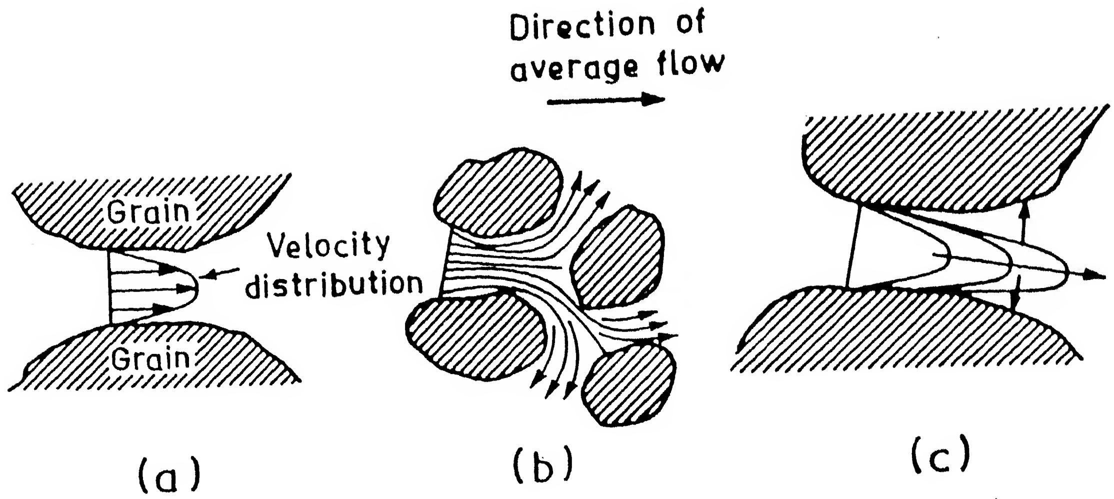


Fig. 1.3. Spreading of pollutant due to mechanical dispersion (a,b) and molecular diffusion (c). (after Bear and Verruijt, 1987).

to mechanical dispersion, (a, b) and molecular diffusion (c) (Bear and Verruijt, 1987). Dispersion of a pollutant originating from a point source at a microscopic scale is shown in Fig. 1.4 (Freeze and Cherry, 1979).

Radioactive decay also causes variation in the concentration distribution of a pollutant in space and time. Adsorption of a pollutant is caused by the interaction of the pollutant with the solid surface of the porous matrix. It may cause clogging of pore spaces and hence, hindering the movement of the dissolved constituents.

Groundwater withdrawal (pumping) can alter the existing concentration distribution of a pollutant. Recharge (injection) through a well and leakage through a leaky layer in the aquifer system also cause changes in the concentration distribution. The change in the concentration distribution is dependent on the quality of water entering into an aquifer system as recharge and leakage, and also the rates of recharge, leakage and pumping.

In an ideal homogeneous and isotropic porous medium with a steady uniform flow system, if only advective transport is considered or predominant, no diminution of concentration occurs. The front of the pollutant distribution remains straight and moves at the rate of groundwater flow. Due to dispersion, some dissolved pollutant actually moves faster and some slower than that would have been expected if only advective transport were considered. Thus, the front of the pollutant distribution appears as smeared instead of

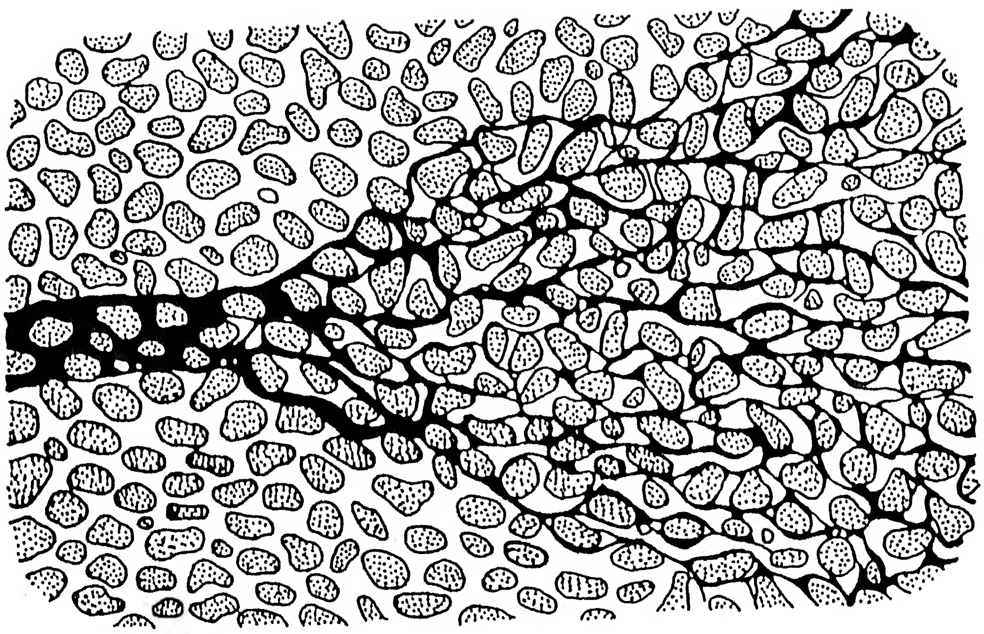
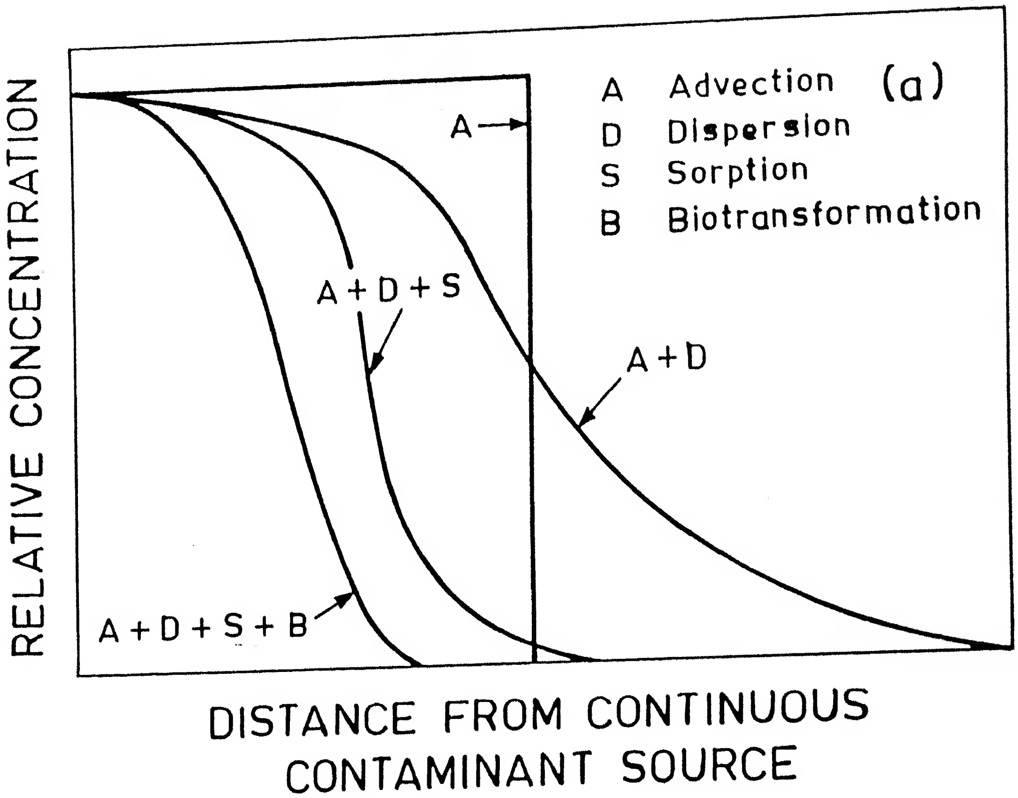


Fig. 1.4. Dispersion of a pollutant originating from a point source at a microscopic scale. (after Freeze and Cherry, 1979)

straight. Fig. 1.5a illustrates the effects of advection, dispersion, sorption, and biotransformation on the movement of a concentration front emanating from a continuous contaminant source (Barcelona et al. 1988). The combined effects of the advection, dispersion, sorption and biotransformation on the movement of a concentration front emanating from an intermittent contaminant source is shown in Fig. 1.5b (Barcelona et al. 1988). Fig. 1.6 shows the difference in breakthrough curves in one dimensional flow through a porous medium if dispersion is also considered with advection.

In uniform laminar flow, contours of constant concentration remain circular with a radius that increases with time as the pollutant is transported downstream by advection, dispersion and diffusion (Fig. 1.7a). These concentration contours become elliptical in shape in case of uniform groundwater motion. (Fig. 1.7b). It occurs due to presence of porous matrix, heterogeneity in pore sizes, pore spaces and pores configuration. These factors also affect the size of the concentration ellipses. The major axis of the elliptical contours remains parallel to the velocity vector. The length of the major and minor axes of the ellipses are observed to change when the magnitude of the uniform velocity is changed (Hunt, 1983). The size of the ellipses become larger as the pollutant propagates with the flow.

Once the pollutants are released into aquifer, it generally move in the form of a plume. The size and shape of the plume depends



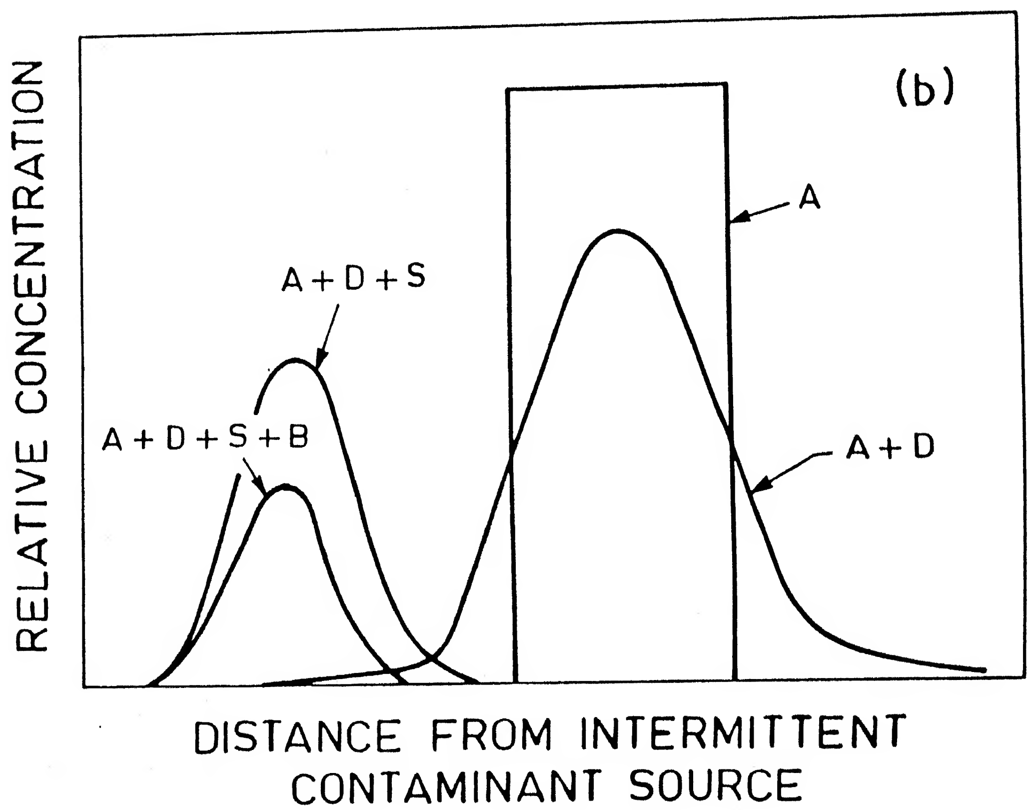


Fig. 1.5. Concentration fronts for (a) continuous source (b) intermittent source (after Barcelona et al, 1988).

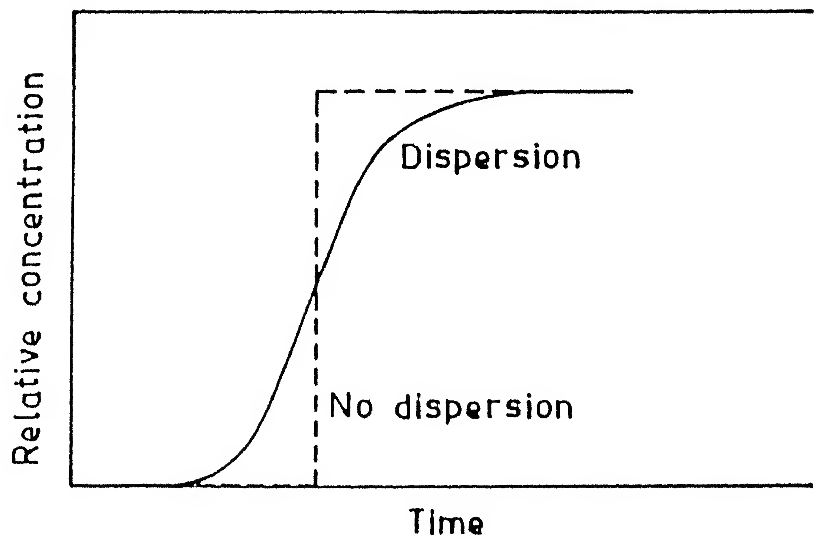


Fig. 1.6 Breakthrough curve in a one dimensional flow.

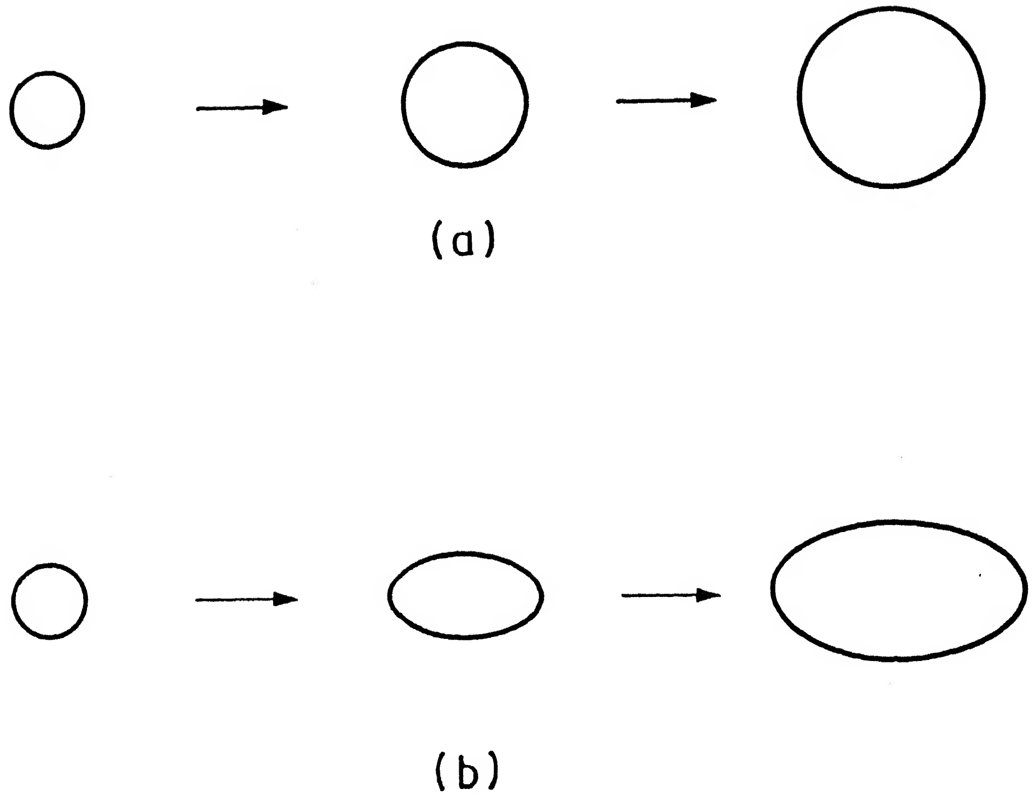


Fig. 1.7 Contours of constant concentration in (a) uniform laminar fluid motion and (b) uniform groundwater motion (after Hunt, 1983).

on local geology, pollutant concentration, pollution release rate, nature of pollutant, and flow characteristics. Fig. 1.8 shows some of the possible changes in the size and shape of the plume (Barcelona et al. 1988). Plume enlargement results from an increase in the rate of waste discharge to the groundwater system. Similar effects occur if the retardation capacity of the geologic materials is exceeded, or if the water table rises closer to the source, causing an increase in dissolved pollutant concentration. Decrease in waste disposal, lowering of the water table, retardation through sorption and reduction in groundwater flow rate can diminish the size of the plume. Nearly stable plume configurations occur if the rate of waste release is steady with respect to retardation and transformation processes. A plume shrinks in size when pollutants are no longer released to the groundwater system or when a mechanism to reduce pollutant concentration is present. An intermittent or seasonal source produces a series of plumes which are separated due to advection that continues even during intervals between pollutant releases. Additional factors including local or regional groundwater stresses such as pumping or recharge and local or regional influences such as aquifer permeability, leakage etc. cause an appreciable change in the size and shape of the pollutant plume. The resulting plumes may be irregular in shape.

In a strict sense, any impurity present in the groundwater can be called a contaminant. Generally, when the concentration of this contaminant exceeds a specified or standard limit so that the

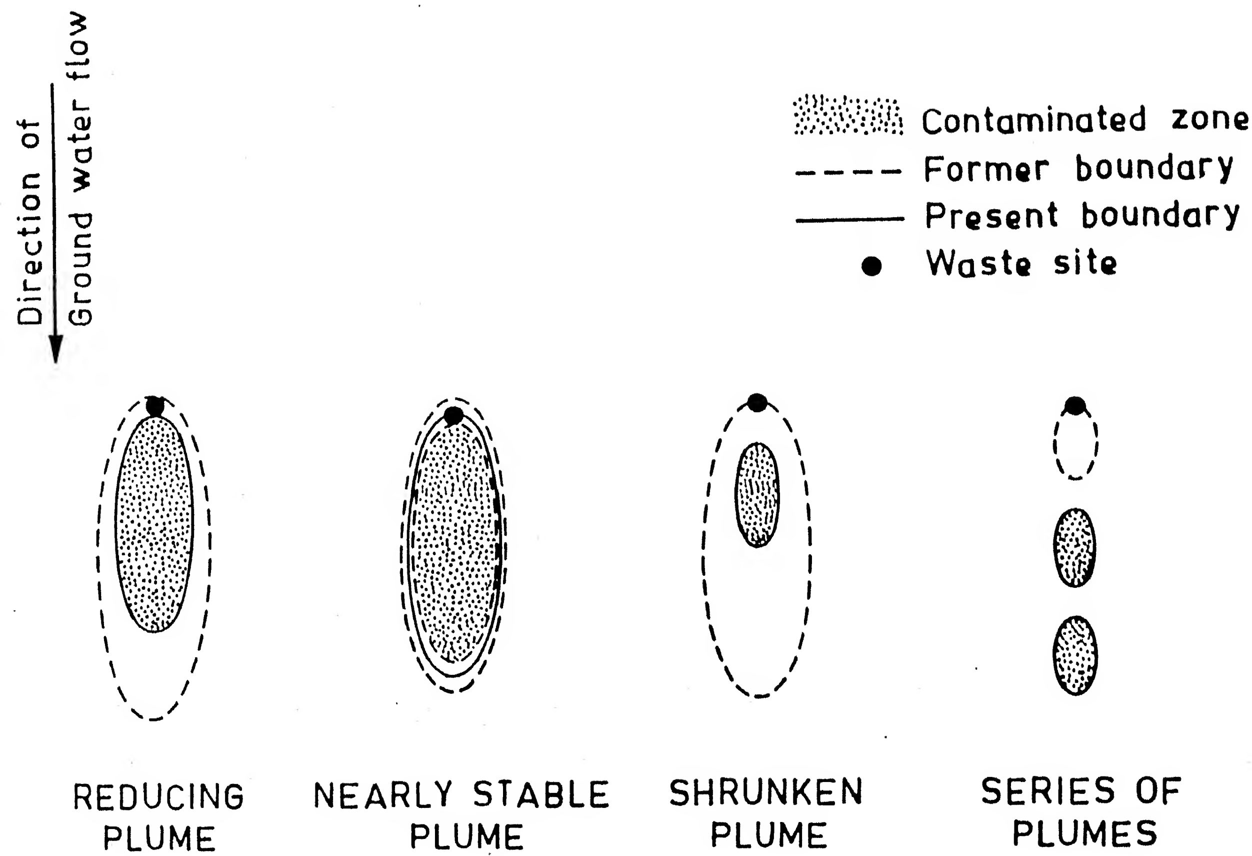


Fig. 1.8. Various plume characteristics (after Barcelona et al, 1988)

presence of the contaminant is potentially hazardous or objectionable, it is designated as a pollutant. However, in this thesis no distinction has been made between a pollutant and a contaminant partly because, the specified objectionable level has been treated as a variable in the management models.

1.3 OBJECTIVES OF THE THESIS

A threat to the quality aspect of the groundwater system is caused by the industrialization, urbanization and application of agrochemicals in agricultural and horticultural practices. In addition, human activities which are responsible for disturbing the ecosystem and certain natural processes are introducing pollutants to the groundwater system continuously or intermittently. Contamination of groundwater has become a serious problem in all industrialized, urbanized and even in rural areas because the quality aspect limits the potential use of groundwater resource for various purposes. Now a days, both developed and developing countries are conscious about this acute problem.

The widespread degradation of groundwater quality requires an integrated approach towards management of groundwater quantity and quality on a global, regional, local or an individual well scale. In both developed and developing countries, the optimal allocation of available water resources for various uses while satisfying the objective of ensuring enhanced quality of life in the long run is a

match demand for various purposes and available supplies in a sustainable way. The optimum management can ensure sustainability only when it has a clear picture of the demands and available sources which need to match in all respects such as time, location, quality and quantity. Keeping these factors in view, the present work has been carried out. The specific objectives of this thesis are as follows:

1.3.1 Specific objectives

(1) Formulation of a constrained nonlinear optimization model for regional integrated management of groundwater pollution and groundwater withdrawal using embedding technique

(2) Development of methodologies to implement nonlinear programming techniques such as Hooke-Jeeves and Powell conjugate direction algorithms in conjunction with exterior penalty function method for solving the constrained nonlinear optimization problems

(3) Performance evaluation of Hooke-Jeeves and Powell conjugate direction algorithms for solution of the integrated management model

(4) Evaluation of management strategies for prescribed management problems under different management scenarios depicting various specified boundary conditions, various physical and geological conditions, and other managerial constraints

(5) Comparison of the suitability of the two algorithms in terms of accuracy, efficiency, ease and feasibility in computing, and

robustness for the solution of the integrated management model

(6) Extension of the integrated management model to include multiple objectives of management and application of the constraint method to obtain Pareto-optimal solutions for the multiobjective optimization model.

Four groundwater management problems are considered for the analyses. They are: (1) Integrated management for groundwater supply, (2) Integrated management for groundwater remediation, (3) Radionuclide pollutant management, and (4) Special case of Quantity management. All these problems are based on two models, Model I and Model II. Model I is a maximization problem. It aims at finding the maximum pumping from the entire aquifer within a planning horizon to satisfy various demands for water of desired quality. Model II is a minimization problem. It aims at finding the minimum pumping from the entire aquifer, in a planning horizon to contain the pollution plumes, or to restore the aquifer upto desired quality for various uses. The special case of quantity management which deals with quantity aspect only is considered to evolve the policies when pollution free aquifer is assumed or the quality aspect is irrelevant. This study is also carried to assess the computational difficulties in solving the management models if quality aspect is also blended in a single framework.

The discretized equations of the coupled set of flow and solute transport equations appear as equality constraints in the optimization model. In addition to these simulation constraints,

managerial constraints like restrictions on hydraulic heads, pumping, pumping locations and concentration appear as inequality constraints in the optimization model. The models are solved for three types of boundary conditions, namely: (i) Dirichlet type, (ii) Neumann type, and (iii) Cauchy type. These boundary conditions act as physical constraints.

The effect of uncertainties in parameter estimates is illustrated by considering deterministic and random modeling of hydraulic conductivity as different management scenarios. The physical conditions such as leakage and artificial recharge are also designated by different management scenarios.

Product of decision variables defining concentration and velocity fields occurs in the advective and dispersive transport terms of the simulation constraints. Therefore, the integrated management model becomes nonlinear. Due to the complex nature of the nonlinearity and difficulty in finding derivatives, nongradient based nonlinear programming techniques such as Hooke-Jeeves and Powell conjugate direction methods are employed to solve the resulting unconstrained minimization problems.

1.4 ORGANIZATION OF THE THESIS

Besides this introductory chapter, this thesis contains eight more chapters. Chapter 2 is devoted to the review of existing literature relevant to optimal groundwater management problems. Some of the generic issues of modeling transient groundwater management

problems are also discussed along with the motivation of the thesis.

Chapter 3 describes mathematical modeling of the integrated regional groundwater management problem. The description of the flow and transport equations in a leaky confined aquifer system, and discretization of these differential equations using finite difference method are presented. This chapter also deals with the constitutive equations for the flow and transport processes. The formulation of the optimization model for the groundwater management problems, concept of exterior penalty function method along with the sequential unconstrained minimization formulation, and solution techniques using pattern search methods are described. The dimensionless numbers; Reynolds number, Courant number and Peclet number are also discussed in order to validate the assumptions inherent in the modeling.

Chapter 4 deals with the application of nonlinear programming techniques to solve the groundwater management models. Various methods available to solve the unconstrained optimization models are discussed in the context of groundwater management problems. The algorithms of Hooke-Jeeves method and Powell conjugate direction method are described in detail in this chapter. The modifications necessary in order to implement these algorithms for the solutions of groundwater management problems are also described.

Performance evaluation of the implemented algorithms are presented in Chapter 5. Solutions of some standard mathematical problems that were obtained using the coded algorithms to test the

correctness of the developed computer codes are presented. The convergence of optimal solutions for groundwater management problems and the global optimality of the solutions are discussed. The effect of discretization due to varying time intervals and grid sizes are also analyzed. The applicability of the implemented algorithm to larger study area is also explored and discussed in this chapter.

Optimal solutions for various groundwater management problems under different management scenarios based on different boundary conditions; and physical, geological, managerial and other local constraints are presented in Chapter 6. The problems considered for the analyses are: (1) Integrated management for groundwater supply, (2) Integrated management for groundwater remediation, (3) Radionuclide pollutant management, and (4) Special case of Quantity management. Results for the special case of quantity management are presented to analyze a groundwater extraction problem when pollution free aquifer is assumed or the quality aspect is irrelevant. Results for this case are utilized to assess the complexity in solving the management model and impacts on the management policies, if quality aspect is conflated. The limitations and global optimality of the results are also discussed.

Chapter 7 presents a comparison of Hooke-Jeeves and Powell conjugate direction algorithms for the suitability of solution of groundwater management problems. Some computational difficulties encountered in the modeling and their remedies are also discussed in addition to the model limitations and global optimality.

Chapter 8 deals with the extension of single objective optimization problem to multiobjective optimization problem. The formulation of multiobjective optimization problem encountered in groundwater management and its solution techniques are described. A set of Pareto-optimal solutions obtained for the two-objective model is discussed.

Chapter 9 focuses on the summary and conclusions of this study. Scope for future work is also discussed.

The structures of the computer programs developed and used in the present study are appended at the end in Appendix I.

LITERATURE REVIEW

CHAPTER 2

LITERATURE REVIEW

Since the mid-1960s, numerical models have been used extensively for the management of groundwater resources. Numerical simulation models representing the complex real-world systems provide limited information regarding the response of the system and the possible hydrologic, environmental or economic tradeoffs. Such models are executed systematically and repeatedly under various design scenarios to achieve a particular objective. Use of such an approach often sidesteps rigorous formulation of groundwater management goals and fails to consider important physical and operational restrictions (Gorelick, 1983). In contrast, optimization models can identify optimal planning, design or operational policies within the context of the systems quantifiable objectives and hydrologic, physical, economic and environmental constraints. The blended use of simulation and optimization components such as the one presented in this thesis enables the groundwater

hydrologists to model the complex real-world systems more adequately over the operating range of interest while formally incorporating specific objectives and constraints of management.

The simulation component can be linked with the optimization model via either embedding or response matrix methods. The Embedding Technique (ET), first presented by Aguado and Remson (1974) directly incorporates the numerical approximations of the governing equations as constraints in an optimization framework. The Response Matrix (RM) technique is based on the superposition principle and linear systems theory. It utilizes unit responses obtained from an external simulation model to describe the influence of a unit stimulus on the decision variables. An ensemble of the unit responses in the form of a matrix is included in a management model. This particular approach and analogous approaches utilizing linear system characteristics were first proposed for petroleum management by Lee and Aronofsky (1958), and Wattenbarger (1970). Later on, many researchers (Maddock, 1972, 1974; Maddock and Haimes, 1975; Morel-Seytoux and Daly, 1975; Schwarz, 1976; Haimes and Dreizin, 1977; Heidari, 1982; Herrling and Heckele, 1986; Peralta and Kowalski, 1986; Tung, 1986; Reichard, 1987; Peralta et al., 1988a, 1988b, 1990) employed this approach to groundwater management problems. Detailed discussions on these two methods are available in Gorelick (1983) and Peralta et al. (1991).

Many other researchers have reported application of optimization techniques for groundwater quality and quantity

management. Aguado et al. (1974) determined the optimal steady state pumping scheme to maintain groundwater levels below specified elevations for a dry dock excavation site. The ET was used and the linear finite difference form of the Boussinesq equation was employed. Later on Aguado and Remson (1980) introduced setup costs in the study by reformulating the problem as a fixed charge problem where costs due to pumping plus the fixed costs due to well installation were considered. Critical discussions on this study are available in Elango (1981), Padmanabhan (1981), and Evans and Remson (1982). Cummings and McFarland (1974) presented a groundwater management model using approaches other than distributed parameter models particularly applicable to salinity control.

Alley et al. (1976) formulated a transient aquifer management model using embedding technique and finite difference approximations of the flow equation for confined aquifer system. They maximized hydraulic heads while obtaining a specified flow rate from wells within the system. The transient behaviour was treated by successive management models, one for each time step. The optimal solution from one time step was treated as initial condition for the next management model.

Willis (1976a) formulated the steady state management of waste disposal activities in aquifers as Linear Programming (LP) problem. The objective was to minimize the cost of surface water treatment while maintaining the water quality at supply or recharge wells. He considered only advection and linear kinetic decay terms in the

constraints placed upon the exogenous water demands.

Molz and Bell (1977) introduced the concept of optimal hydraulic gradient control in the aquifer. They embedded the finite difference approximation of the groundwater flow equation into a linear programming formulation. This model was solved to determine the smallest pumping rate to achieve a steady state to ensure the stationarity of fluid stored in the aquifer.

Gorelick et al. (1979) recognized the problem of storing and manipulating a large time and space discretized embedded simulation matrix. To overcome this dimensionality problem he developed an alternate method to solve the transient management problems. A recursive pollutant source management formula was developed for the determination of maximum permissible concentration in a river with stream aquifer connection, keeping the crop chloride tolerances at agricultural supply wells within the permissible limit. This method is applicable to a case where the concentrations throughout the system can be expressed as a function of a single parameter.

Willis (1979) developed a model for aquifer management involving waste injection control, conjunctively managed for supply and quality. He decoupled the management model into hydraulic management component and pollutant source management component. Both the components were solved as separate LP problems. To handle long time frames, he discretized the partial differential equations over space only using FEM. The analytical solutions to these resulting systems of space discretized ordinary differential equations were

included as embedded constraints.

Remson and Gorelick (1980) demonstrated the use of embedding approach to control hydraulic gradient in order to contain a plume of contaminated groundwater. The steady state management model formulated as a linear program was solved to obtain optimal well locations and their minimal pumping or recharge rates.

Ben-Zvi and Bachmat (1980) considered the task of planning the operation of a groundwater reservoir. They proposed an algorithm to improve an existing plan on the basis of available information. The algorithm consists of three stages, i.e., (i) Deterministic stage: The planner ignores uncertainties as if the necessary information were fully known, and thus variance of the input to the decision making model is zero. (ii) Risk with known statistical model and parameter values: The planner generalizes the model by taking into account the fact that some elements of the input are random. However it is assumed that the distribution is known and stationary, and the parameters of the distribution are known as if the data samples pertinent to the input were infinitely large. (iii) Risk with parameter estimates: The planner further generalizes the decision making model by taking into account that, because of finite data sample, one can only estimate the distribution parameters.

Alkan and Shamir (1980) employed multiobjective optimization method to plan the development and seasonal operation of a regional water resources system. They considered an arid region in the south of Israel. Six objectives were considered for the planning problem.

Spatial and temporal variations in demand and supply of water were considered.

Elango and Rouve (1980) formulated the groundwater management model as linear program using FEM to discretize the flow equation. They incorporated the simulation constraints into the optimization model using embedding technique. The model was solved for quantity management only and it was realized that computational difficulties might arise when a large number of equality constraints are considered.

Vedula and Rogers (1981) formulated a linear programming model, not applicable for groundwater system, for four-reservoir system to find optimum cropping patterns under the restrictions on land, water and downstream release. The model was applied to the Cauvery river basin, India. Two objectives, maximizing net economic benefits and maximizing irrigated cropped area were analyzed in the context of multiobjective planning, and the associated tradeoffs were discussed.

Gorelick and Remson (1982a) employed the ET for the steady state pollutant source management problem. FDM was used to discretize the solute transport equation. This model maximizes the waste disposal at two locations while protecting water quality at supply wells and maintaining an existing waste disposal facility. They also considered the identification of the most suitable waste disposal sites in a study area. The linear programming formulation was arranged and scaled so that the linear programming dual

variables, which represent sensitivity coefficients, served as unit source impact indicators.

Gorelick and Remson (1982b) used RM method to manage waste disposal activities over a period of several years in such a way that solute concentrations at supply wells would never exceed water quality standards even after waste disposal activities had ceased. They illustrated the model with an one-dimensional transient case involving multiple sources of groundwater pollution, and maintenance of water quality at water supply wells over all time.

Gorelick (1982) utilized the Method of Characteristic (MOC) based solute transport model of Konikow and Bredehoeft (1978) as a linear component to generate the response matrix in a pollutant source management model applied to a complex hypothetical regional aquifer. He demonstrated that the solution of large scale and long time frame management problems could be solved by using a numerically stable implementation of the revised simplex method (Saunders, 1977).

Bredehoeft and Young (1983) considered the conjunctive use of groundwater and surface water for irrigated agriculture. The influence of uncertain surface water supply on the net revenue from the crops was computed. The management modeling approach illustrates quantitatively that the development of groundwater systems may be motivated by a desire to insure against periodic short water supplies. Management models on conjunctive use of groundwater and surface water are also discussed in Chaudhary et al. (1974), Taylor

and Luckey (1974), Yu and Haimes (1974), Morel-Seytox (1975) and Haimes and Dreizen (1977).

Gorelick et al. (1983) utilized two approaches, linear programming and multiple regression combined with solute transport simulation to identify the locations and magnitudes of groundwater pollutant sources. They illustrated the model for both steady state and transient management problems.

Gorelick et al. (1984) formulated the aquifer reclamation design as a Nonlinear Programming (NLP) problem. They combined a finite element transport simulation model, SUTRA (Voss, 1984) with a nonlinear optimization procedure. Optimization was accomplished using a projected Lagrangian method with a modified quadratic penalty function. The computer code MINOS (Murtagh and Saunders, 1980) was used for this purpose. The methodology was demonstrated for both steady state and transient contaminant migration problems. They however, realized that as with any nonlinear nonconvex optimization problem, global optimality is difficult, if not impossible to guarantee.

Atwood and Gorelick (1985) considered containment and removal of contaminant plume. They decoupled the management problem and reduced it to one of hydraulic gradient control. The optimal well locations and their pumping or recharge rates were obtained to keep the hydraulic gradient near zero around the shrinking plume.

Lekoff and Gorelick (1986) considered the problem of contaminant plume isolation and removal using hydraulic gradient

control. They accounted for chemical retardation of the migrating contaminants and studied the impact of treatment process costs (a linear objective) versus pumping costs (a quadratic objective) on the optimal design of a rapid aquifer restoration systems.

Datta and Peralta (1986a) considered groundwater contaminant containment problem. They used embedding technique and developed an influence coefficient for the optimal modification of regional steady state potentiometric surface design.

Datta and Peralta (1986b) presented a multiobjective optimization procedure for developing a regional conjunctive water management strategy for an important rice production area in Arkansas, U.S.A. The objectives considered were : (a) minimization of the total cost of water use and (b) maximization of total withdrawal from the aquifer. They also accounted for the opportunity cost due to the loss in agricultural production caused by nonavailability of water.

Tung (1986) developed a chance constrained groundwater management model for an idealized confined aquifer system incorporating the analytical equations for groundwater flow using the unit response function derived from the Cooper-Jacob equation. Random nature of transmissivity and storage coefficient were considered explicitly. The objective was to determine optimal pumping pattern in a well field subjected to a specified system performance reliability. Applicability of the model was illustrated for a hypothetical study area.

Ahlfeld et al. (1986) considered the design of optimal strategies for contaminated groundwater remediation. They formulated a NLP model and illustrated the working of the model for both steady state and transient management problems. The computer code MINOS was used. It was realized that computational cost was appreciable because of repeated subroutine calls for function and Jacobian evaluations.

Jones et al. (1987) developed a Differential Dynamic Programming (DDP) model for transient unconfined flow. Optimal solution was obtained for the management problem dealing with quantity aspect only.

Yazicigil and Rasheeduddin (1987) considered a hydraulically connected multiple aquifer system. They formulated the management model as linear program and determined optimal extraction schedules satisfying target values.

Ahlfeld (1987) presented a method for improving the solution efficiency of a NLP model for groundwater management by evaluating the Jacobian analytically by using the adjoint sensitivity method rather than evaluating it numerically. He demonstrated this approach for the Woburn aquifer.

Gorelick (1987) studied the impact of spatial variability in hydraulic conductivity upon optimal groundwater contaminant capture curve design. He used Monte Carlo analysis to incorporate the uncertainties. Synthetic hydraulic conductivity maps were generated assuming an exponential correlation structure. Optimal well layouts

and pumping rates were determined for each hydraulic conductivity realization.

Wagner and Gorelick (1987) incorporated parameter estimation uncertainties into the decision making process for optimal groundwater quality management. They explicitly incorporated parameter estimation uncertainties into a chance-constrained formulation for the aquifer remediation design problem. FEM was used to discretize the flow and transport equations. Optimal solutions were obtained using nonlinear stochastic programming. Ahlfeld et al. (1988) considered the remediation design of contaminated groundwater and formulated the problem as an NLP.

Bogacki and Daniels (1989) presented a FEM based NLP problem, resulting from the coupled set of flow and convection-dispersion equations. This model finds minimal extraction rates and optimal well locations for aquifer clean up problems. The objective function considered was linear. Solution was obtained by using Lagrangian multipliers. The embedding technique was used to incorporate the simulation model within the optimization model.

Mahon et al. (1989) used the MINOS optimization algorithm (Murtagh and Saunders, 1987) and demonstrated stability of the embedding technique for a larger sized study area, 13000 square miles using over 1600 constraints. However the application was demonstrated only for steady state quantity management problems.

Peralta and Datta (1990) employed embedding technique to medium sized study area to determine optimal steady state regional

groundwater use strategies. Peralta and Ward (1991) compared multiobjective strategies and models for optimizing the short term containment of a 2-D groundwater contaminant plume. They considered two types of objectives, hydraulic and economic, and used Weighting Method (WM) to convert the two objective problem into a single objective optimization model. The response matrix approach was used in the formulation of the optimization model. The optimal pumping strategies were obtained for both steady state and transient management problems.

Cleveland and Yeh (1991) developed an algorithm for the optimal configuration and scheduling of an aquifer tracer test for estimating the transport parameters. The goal was to maximize a measure of the information matrix without exceeding a budget.

Lee and Kitanidis (1991) presented a model for optimal aquifer remediation having limited information. They employed embedding technique to incorporate flow and solute transport equations. However, simulation equations were discretized over space only and analytical solutions for time derivatives were obtained to embed the simulation equations as constraints into the optimization model. The probabilistic approach was used to account for uncertainty. The objective was to find the most cost-effective management policy for aquifer decontamination. The policies were expressed as sum of a deterministic and a stochastic control term. The former was obtained by solving deterministic optimization problem through constrained differential dynamic programming, and the latter was obtained by a

perturbation approximation to the stochastic optimal control problem. The applicability of the model was illustrated for a hypothetical aquifer.

Finny et al. (1992) developed NLP based combined simulation - optimization model for the control of saltwater intrusion in the Jakarta multiple aquifer system. The optimization model incorporates a quasi-three-dimensional finite difference simulation model of the aquifer system. It minimizes the total squared volume of saltwater in each aquifer of the groundwater system under the restriction placed upon water demand in the basin. Parametric programming was used to determine the tradeoffs affecting the optimal decisions.

Yeh (1992) presented a review on the systems analysis and optimization techniques developed in the field of water resources for the planning and management of a groundwater system. The areas covered were groundwater management models, inverse solution techniques for parameter identification and optimal experimental design methods. However, the emphasis was placed upon groundwater supply management models dealing with quantity aspect only.

Latinopoulos et al. (1994) formulated the steady-state management model for groundwater remediation problem as linear and quadratic programming models. They used response matrix approach to incorporate finite difference approximation of groundwater flow equation, and employed MOC based solute transport model (Konikow and Bredehoeft, 1978) to compute contaminant distribution in a post optimal stage. They focused mainly upon sensitivity analysis for the

aquifer transmissivity. The applicability of the model was illustrated for a hypothetical aquifer. The solutions were obtained using MINOS (Murtagh and Saunders, 1987).

Ritzel et al. (1994) employed a newly growing search technique, Genetic Algorithm (GA) to a multiple objective groundwater pollution containment problem. The objectives considered were : (1) maximize reliability, and (2) minimize cost. The tradeoff curve was obtained between these two objectives. They utilized response function approach, and optimization and simulation models were linked externally. The results were compared with that obtained by Mixed Integer Chance Constrained Programming (MICCP) developed by Morgan et al. (1993).

Wang and Ahlfeld (1994) formulated a nonlinear management model for the optimal design of aquifer remediation strategies in which the well location problem was solved by explicitly incorporating the spatial coordinates and pumping rates of wells as decision variables. The Hermite interpolation function is used to represent the well location. They used embedding technique to incorporate the coupled set of Galerkin finite element discretization of the flow and transport equations. Two types of formulation: (i) fixed well formulation, and (ii) moving well formulation were presented. The applicability of the model was evaluated for a hypothetical aquifer assuming homogeneous, isotropic and confined with no leakage. MINOS was used to solve the nonlinear optimization problem.

It is evident from the above discussion that substantial

research has been done on the applicability of optimization techniques to groundwater management problems. However, it is evident that majority of these management models used the simplifying assumptions of linear systems and restricted the models to linear objective functions and constraints. Comparatively less attention has been provided to accurate modeling of the nonlinearities especially inherent in the solute transport process and in unconfined aquifers. Nonlinear objective functions and constraints were less frequently used also. It is no doubt simpler to model a linear system incorporating linear objectives and linear constraints. However, many realistic problems may require modeling the inherent nonlinearities, while incorporating nonlinear managerial or other constraints and objectives. It is also apparent that the increasing computing powers of modern day computers have made it feasible to model large nonlinear systems and to use NLP algorithms. Recent studies are increasingly dealing with management of large groundwater systems using NLP algorithms.

Research and literature are relatively scarce on groundwater quality management models involving nonlinear constraints and objectives. It should be noted that no large scale application of the embedding technique has been reported for the transient groundwater pollutant management models. Gorelick (1983) reported in his classic review paper that the application of embedding technique has revealed that numerical problems arise in utilizing the commercial linear programming packages (Evans and Remson, 1982;

Gorelick, 1980). However, solutions have been obtained for small problems. For larger systems, solutions may be difficult to obtain. Computational problems are much more severe when NLP algorithms are used.

Integrated management models that deal with groundwater withdrawal and pollution within the same framework by incorporating the coupled set of flow and transport equations into the optimization model are becoming computationally feasible. Nonlinear models are more realistic for adequately describing the effects of advection, dispersion, diffusion and decay phenomena on contaminant migration. Nonlinear management models are necessary to consider the nonlinear objectives and constraints encountered in the real life situations. Literature and research are also scarce on multiobjective nonlinear optimization models. It is evident from the above discussions that multiobjective optimization models dealing specially with groundwater system are rare.

Another aspect that must be emphasized is the incorporation of errors and uncertainties in the modeling process, in order to enhance the reliability of groundwater management models. Heterogeneity, anisotropy, spatial nonuniformity and sometimes temporal variability of certain hydrologic parameters used in modeling flow and transport processes must be accounted for in a model. Uncertainties and errors in estimating these parameters must be incorporated in the decision making process. These aspects also received inadequate attention of researchers.

The study reported in this thesis is motivated by the observations mentioned above. The goal is to formulate, develop and test an integrated groundwater management model for groundwater withdrawal and pollution control. Again, discretized governing equations for the flow and transport processes are incorporated directly in the optimal management model. These resulting nonlinear optimization models use NLP algorithms for solution. The performance evaluation of the developed model and the NLP algorithms used for solution is necessary to establish the feasibility of these approaches. Development of these management models and the NLP algorithms used for solution are discussed in the following chapter.

MATHEMATICAL MODELING OF REGIONAL GROUNDWATER MANAGEMENT PROBLEMS

CHAPTER 3

MATHEMATICAL MODELING OF REGIONAL GROUNDWATER MANAGEMENT PROBLEMS

Mathematical modeling of regional groundwater management problems involves the formulation of the management model, its development, solution, validation and interpretation of the solution results to establish its applicability. In addition, the sensitivity of the model needs to be analyzed with respect to uncertainties associated with aquifer parameter estimates, initial and boundary conditions, and other information required for modeling. Fig. 3.1 shows the salient features of a groundwater management system applicable to various kinds of groundwater management problems encountered in real life situations.

Formulation of the management model requires the establishment of the system boundaries and domain, incorporation of the coupled set of flow and transport equations, estimation of system parameters

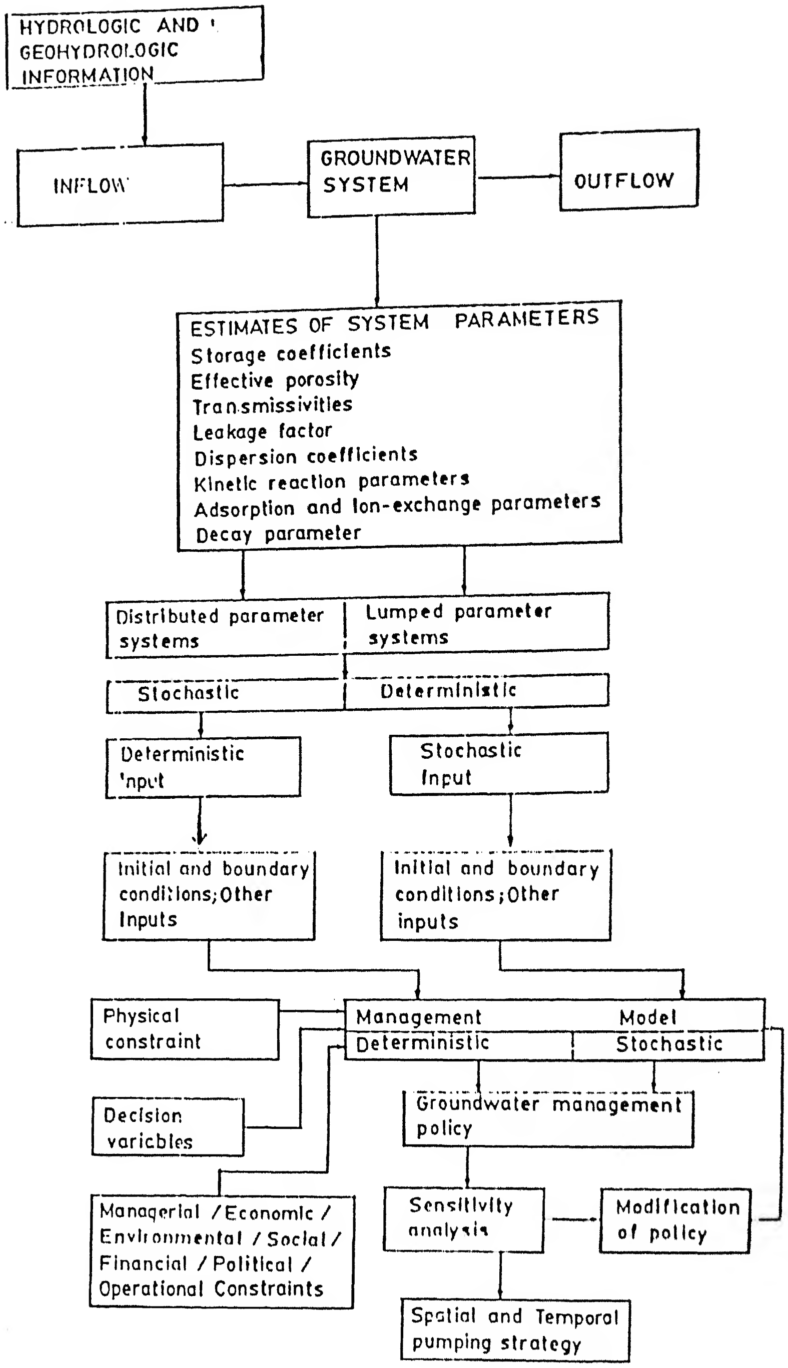


Fig. 3.1 Salient features of a groundwater management system

and other system information required for the description of the physical processes, selection of decision variables, constitution of desired objectives, and imposition of system constraints and performance criteria. In the formulation of the model, it is necessary to identify all significant aspects of the groundwater system under consideration that must be included. Identification of the assumptions that are necessary to approximate a real-world system by a mathematical model are essential to decide the form in which the model will be cast, the level of model details and the manner in which the model will be utilized. These decisions play vital roles in the model formulation.

Generally, a simplified model may be formulated as a first step. Then the model is developed successively to incorporate all possible details and adequate descriptions of various phenomena occurring within the groundwater system under consideration. The process of developing the model continues with the advancements in theoretical descriptions of the involved processes, computational methods and computing powers. Subsequent developments of the model incorporate various constraints required to make the policies economically, financially, socially, environmentally and politically feasible in addition to operational and other technical constraints.

After the development of the model, the solution techniques are analyzed for the suitability of the solution of the model. Depending upon the nature of the model, proper optimization methods are employed to evaluate the performance of the model.

The validity of the model is tested by evaluating the performance of the model in solving a groundwater management problem under consideration. Before evaluating the performance of the model, the coded algorithms are tested for its correctness by finding the solutions of some test problems for which exact solutions are either known or reported by some other researchers. The model is also checked for infeasibility if any, due to ill formulation.

Solutions can be obtained for different management scenarios that are designed depending upon the goal of the whole study. These scenarios may be reflected by different imposed boundary conditions, different methods for incorporating parameter estimation uncertainties, different aquifer environment, and various physical and managerial constraints.

The management policies are evolved for various management scenarios. The consequences of the policies are interpreted in terms of physical happenings within the system. The various tradeoffs involved are evaluated to aid the decision making process involving more than one objective.

Applicability of the model is evaluated for the suitability, ease, robustness, accuracy, efficiency and computing feasibility. Various models should be evaluated on the basis of not only structure, but also on the basis of its adequacy in approximating the behaviour of the real world system over the operating range of interest. Other criteria for solution of a model are the suitability of the methods adopted for solution and accuracy of the solution.

If accurate and realistic formulation of the model is not achieved, no matter how detailed and complex the model is, solutions of the model will yield physically meaningless and inapplicable results. Therefore, solution results from such models can not constitute a real system optimum. The decision or management model should be formulated as a nonlinear one if the physical, chemical and biological processes occurring within the system are nonlinear in nature, or the objectives or constraints encountered in the planning problem are of nonlinear nature. However, the nonlinear models are generally difficult to solve. Therefore, linear models approximating the inherent nonlinearities are frequently used to reduce the computational burden. Moreover, it should be emphasized here that the accuracy itself often can not be assessed precisely. The selection of appropriate model requires a subjective judgment and a feel for the behaviour of the real world system. It may happen that one model may be more accurate than a competitive formulation over one subregion and for a given management scenario, but less accurate over another subregion or for a different management scenario.

To sum up, development and selection of a mathematical model is partially subjective in nature. One has to decide based on the relative assessment of the structure, accuracy, applicability, efficiency and economy in terms of both time and money. The uncertainties inherent in accurate modeling of the physical processes, and in the prediction of future impacts of various

management decisions are other complexities, that should be considered.

3.1 GROUNDWATER SYSTEM

A mathematical model describing the groundwater system must incorporate the following aspects:

(i) geometry of the aquifer boundary and its physical domain under investigation (large scale, smaller scale or individual well project)

(ii) nature of the porous medium (heterogeneity, anisotropy, porosity, hydraulic conductivity, storativity)

(iii) mode of flow in the aquifer (3-dimensional, 2-dimensional or 1-dimensional)

(iv) flow regime (laminar or turbulent)

(v) relevant state variables and the area or volume over which the averages of such variables are taken

(vi) sources and sinks of water and of relevant pollutants within the aquifer domain and on its boundaries (point or distributed sources and sinks)

(vii) boundary conditions of the aquifer domain under investigation (Dirichlet, Neumann, Cauchy)

(viii) initial conditions for the flow and transport processes (in transient cases)

(ix) nature of pollutant (conservative, radioactive, degradable or adsorbent)

(x) dispersivities

The essential components of a mathematical model simulating flow and transport processes in an aquifer are:

(i) definition of the geometry of the considered domain and its boundaries

(ii) equations governing the flow and transport processes incorporating constitutive relationships (Darcy's law, Fick's law, decay law, adsorption isotherm, law of mass action)

(iii) initial conditions for the flow and transport processes (in transient cases)

(iv) boundary conditions of the aquifer domain under investigation for the flow and transport processes

The mathematical model representing the groundwater system is described by the partial differential equations for the flow and transport processes along with initial and boundary conditions. To incorporate these simulation equations in the optimization model using embedding technique, the mathematical model is converted into a numerical model by discretization of the governing partial differential equations in space and time. This numerical model which is a part of an optimal management model, simulates and predicts the aquifer response to various applied stresses, contamination histories and management policies.

3.2 CONSTITUTIVE EQUATIONS

There are some constitutive equations which describe the physical, chemical and biological processes within the groundwater system. These constitutive equations are the basic equations which constitute the well known groundwater flow and solute transport equations. With the help of groundwater flow and solute transport equations, the excitation response of the system due to applied hydraulic stresses and pollutant loads are assessed. The major constitutive equations encountered in groundwater systems are flux equation (Darcy's law); advective, dispersive and diffusive flux equations; decay equation; adsorption isotherms; and thermodynamic equilibrium equations. These equations are described in the following sections.

3.2.1 Flux equation

In the continuum approach, subject to certain simplifying assumptions as to the solid-fluid interaction, negligible internal friction in the fluid, and negligible internal effects, the conservation of momentum reduces to the linear motion equation, known as Darcy's law (1956). It is used as a flux equation for fluid flow in porous media. Darcy's law extended for a homogeneous anisotropic medium in 3-dimensional flow of a homogeneous incompressible fluid can be written as (Bear and Verruijt, 1987):

$$[q] = [K]\ [J] \qquad (3.1)$$

Where matrices q, K and J are given by:

$$[q] = \begin{bmatrix} q_x \\ q_y \\ q_z \end{bmatrix} \tag{3.2}$$

$$[K] = \begin{bmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix} \tag{3.3}$$

$$[J] = \begin{bmatrix} J_x \\ J_y \\ J_z \end{bmatrix} \tag{3.4}$$

q_x, q_y and q_z are the components of specific discharge vector, q, and J_x, J_y and J_z are the components of the hydraulic gradient vector, J in the x, y and z directions respectively. K_{xx}, K_{xy}, K_{xz}, K_{yx}, K_{yy}, K_{yz}, K_{zx}, K_{zy} and K_{zz} are nine constant coefficients representing hydraulic conductivity components. In heterogeneous medium, each of these components vary in space. K is a second rank tensor of hydraulic conductivity of an anisotropic medium. Hydraulic conductivity class, (K_c), defined by Equation (3.5), of different types of porous medium is given in Table 3.1 (Bear and Verruijt, 1987).

$$K_c = -\left[2 + \log_{10} K\right] \tag{3.5}$$

Table 3.1 Typical values of Hydraulic conductivity class

Porous media/ Aquifer	K_c
Pervious	- 2 - 2
Semi pervious	2 - 6
Impervious	6 - 11
Good aquifer	-2 - 3
Poor aquifer	3 - 7
No aquifer	7 - 11

K in Equation (3.5) is expressed in m/s. In tensor notation, Darcy's law can be expressed as:

$$q_i = - K_{ij} \frac{\partial h}{\partial x_j} \tag{3.6}$$

Where h is hydraulic head. The specific discharge is defined as the volume of water flowing per unit time, Q, through a unit cross-sectional area, A, normal to the direction of flow. Thus, it can be written as:

$$q = Q/A \tag{3.7}$$

3.2.2 Advective, dispersive and diffusive fluxes

Advective flux of a contaminant is the flux carried by the water at the average velocity. It is due to the bulk motion of the fluid. Mathematically it is expressed as:

$$q_{ca} = C\ v \tag{3.8}$$

Where q_{ca} is advective flux of the contaminant and C is the concentration of contaminant present in the fluid. The average velocity, v, through the pores of the porous medium is defined as:

$$v = q/n_{eff} \tag{3.9}$$

Where n_{eff} denotes the effective porosity of the medium.

The dispersive and the diffusive fluxes of a contaminant are expressed by Fick's law. The dispersive flux is a macroscopic flux that produces spreading or dispersion of a contaminant due to microscopic velocity variations in the pore space. It is expressed as:

$$(q_{cds})_i = - D_{ij} \frac{\partial C}{\partial x_j} \qquad (3.10)$$

Where q_{cds} is dispersive flux of the contaminant and D is the coefficient of mechanical dispersion (convective diffusion). D is a second rank symmetric tensor. The dispersive flux is the average of the product of the fluctuating components of velocity and concentration.

The diffusive flux of the contaminant due to molecular diffusion in a porous medium at macroscopic scale is expressed as:

$$(q_{cdf})_i = - (D_d^*)_{ij} \frac{\partial C}{\partial x_j} \qquad (3.11)$$

Where q_{cdf} is diffusive flux of the contaminant, D_d^* is the coefficient of molecular diffusion in a porous medium. D_d^* is a second rank symmetric tensor and is given as (Bear and Verruijt, 1987):

$$D_d^* = T^* D_d \qquad (3.12)$$

Where T^*, referred as tortuosity, is a second rank symmetric tensor that expresses the effect of the configuration of the water occupied portion of the control volume. D_d is the coefficient of molecular diffusion in a fluid continuum. The molecular diffusion is caused by the variations in contaminant concentration within the liquid phase and it produces an additional flux of contaminant from regions of higher contaminant concentrations to those of lower ones. It occurs even in the absence of bulk flow.

The advective, dispersive and diffusive fluxes are expressed in units of kg m of porous medium/m^3 of water/s. Total flux, q_{ct} in saturated porous medium at microscopic level in units of kg/m^2 of porous medium/s is expressed as:

$$q_{ct} = n_{eff} \, (q_{ca} + q_{cds} + q_{cdf}) \tag{3.13}$$

It is basically a sum of advective, dispersive and diffusive fluxes.

3.2.3 Law of decay

The pollutant or contaminant present in the water or adsorbed on the soil grains may decay constantly. The decay of pollutant may be linear, nonlinear or exponential depending upon the nature of the pollutant encountered in groundwater system. If the pollutant is a radioactive substance, its disintegration is governed by the hypothesis of Rutherford and Soddy. According to this hypothesis:

(i) Every atom of radioactive element is constantly breaking

up into fresh radioactive products with the emission of α, β and γ radiations. The new products have completely new chemical and radioactive properties.

(ii) The rate of decay is spontaneous and can neither be accelerated nor retarded under any circumstances, but is entirely dependent upon the law of chance.

Hence, the rate of decay of a radioactive element at any instant is proportional to the number of atoms present. Mathematically it can be expressed as:

$$-\frac{dN}{dt} \propto N \tag{3.14}$$

$$\text{or } \frac{dN}{dt} = -\lambda N \tag{3.15}$$

Where N is the number of atoms originally present, dN/dt represents the number of atoms breaking in unit time and λ is a constant known as radioactive constant, decay constant, transformation constant, or disintegration constant.

The number of atoms left after time t can be obtained by integrating Equation (3.15). It is given by:

$$N = N_o e^{-\lambda t} \tag{3.16}$$

Where N is the number of atoms left after time t and N_o is the number of atoms initially present. Thus, a radionuclide decays

exponentially with time. The rate of decay of the radioactive substance is usually defined by its half-life period ($T_{\frac{1}{2}}$). The half-life period of radioactive substance is the time in which the amount of radioactive substance is reduced to half of its original value and is given by:

$$T_{\frac{1}{2}} = \frac{\ln 2}{\lambda} \tag{3.17}$$

The amount of radioactive substance is expressed in terms of Curie which gives rise to 3.7×10^{10} disintegrations per second. One curie is also equivalent to 1 gm of pure radium.

3.2.4 Adsorption isotherm

An adsorption isotherm is an expression that relates the quantity of an adsorbed component to its quantity in the fluid phase under isothermal condition. Different adsorbate-adsorbent pairs have different isotherms. The adsorption isotherms are generally grouped into two classes: (i) equilibrium isotherms and (ii) nonequilibrium isotherms. Equilibrium isotherms assume that the quantities of the component on the solid and in the adjacent solution are continuously at equilibrium. Any change in the concentration of one of them produces an instantaneous change in the other. In nonequilibrium isotherms, equilibrium is not achieved instantaneously, but is approached at a certain rate. A number of commonly encountered

isotherms have been suggested by many researchers: Fruendlich, Langmuir, Lindstrom et al., Van Genuchten, Lapidus and Amundsen, Hendricks. The expressions of various types of equilibrium and nonequilibrium isotherms given by these researchers are available in Bear and Verruijt (1987). The most widely used and simplest isotherm is linear equilibrium isotherm. It is a linear form of Freundlich equilibrium isotherm and is given by:

$$F = K_d C \tag{3.18}$$

Where F denotes the mass of the pollutant on the solid per unit mass of solid and K_d is called the distribution coefficient or partitioning coefficient.

3.2.5 Law of mass action

The concentrations of pollutants change appreciably due to chemical interactions involved among components within the liquid. The rate of increase or decrease in the concentration of a pollutant depends upon the rate of reaction. The rate of reaction depends upon temperature, pressure, concentration and catalyst if any. The chemical reaction among the components is governed by the law of mass action. According to this law, the rate of a chemical reaction is proportional to the product of the molar concentrations of the reacting substances. Considering a general hypothetical chemical reaction described by the stoichiometric equation:

$$a\,A + b\,B \underset{k_b}{\overset{k_f}{\rightleftharpoons}} g\,G + h\,H \tag{3.19}$$

At equilibrium, the rate of forward reaction (k_f) is equal to the rate of backward reaction (k_b). At this condition, according to the law of mass action, one gets:

$$K = \frac{[G]^g\ [H]^h}{[A]^a\ [B]^b} \tag{3.20}$$

a, b, g, h ?

where K represents a thermodynamic equilibirium constant and depends upon the temperature. [A], [B], [G] and [H] denote the molar concentrations of the components A, B (reactants); G and H (products) respectively. It should be noted here that in many groundwater situations, equilibrium may not be reached for a long time. Such situations need a prior information about the kinetics of the chemical process involved (Bear and Verruijt, 1987).

3.3 Description of flow and transport equations

In order to develop groundwater simulation models, the basic laws are applied to a specific region rather than to individual masses. This is achieved by the Reynolds transport theorem, also called the general control volume equation which is applicable to any extensive property of the system (White, 1986; Chow et al., 1988). The Reynolds transport theorem states that the rate of change of an extensive property of a system is equal to the sum of the rate

of change of extensive property within the control volume and the excess of efflux over influx of the extensive property. Mathematically for the fixed control volume, it can be expressed as:

$$\frac{d}{dt}\left(B_{syst}\right) = \iiint_{CV} \frac{\partial}{\partial t} \left(\beta\ \rho\right)\ d\upsilon + \iint_{CS} \beta\ \rho\ \left(v\ .\ n\right)\ dA \qquad (3.21)$$

Where B_{syst} and β are extensive and intensive properties of the system respectively. ρ, $d\upsilon$, v, dA and n represent respectively density of fluid, differential volume, flow velocity, differential area and outward normal unit vector on the control surface. CV and CS stand for control volume and control surface respectively.

The flow and transport equations governing the flow and pollutant transport processes in a porous medium are obtained using continuum approach in an Eulerian formulation. These equations are based on the principle of conservation of mass. To analyze the fluid motion and pollutant transport in a porous medium, this basic law is applied to an infinitesimal fixed control volume. These equations are obtained from the Reynolds transport theorem as mentioned earlier.

3.3.1 Groundwater flow equation

Groundwater flow equation is a continuity equation for flow. Fig. 3.2 shows the definition sketch of a leaky confined aquifer system. A control volume having a shape of a parallelopiped of dimensions dx, dy and b is shown in Fig. 3.3. b denotes the

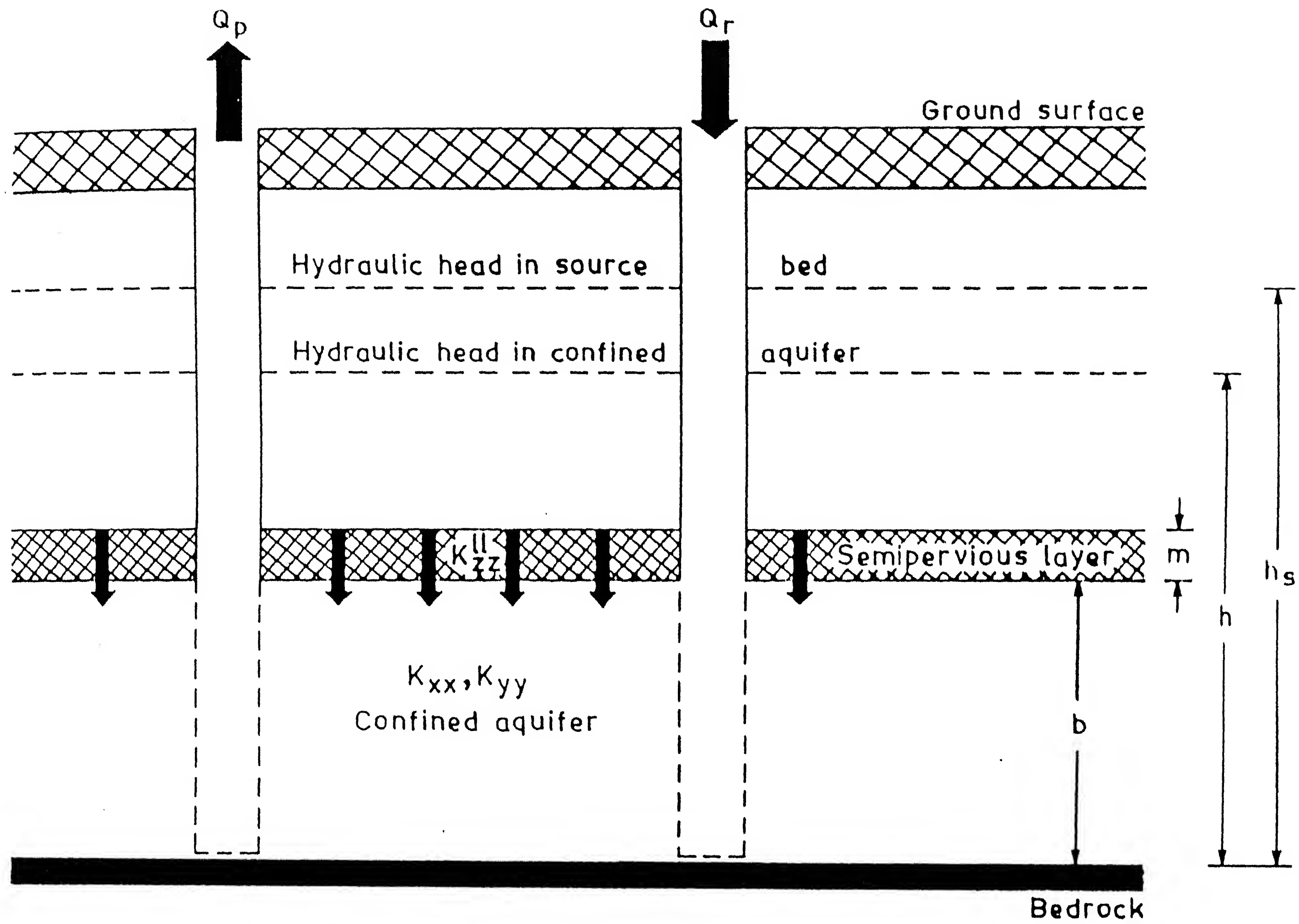


Fig. 3.2 Definition sketch of a leaky confined aquifer system.

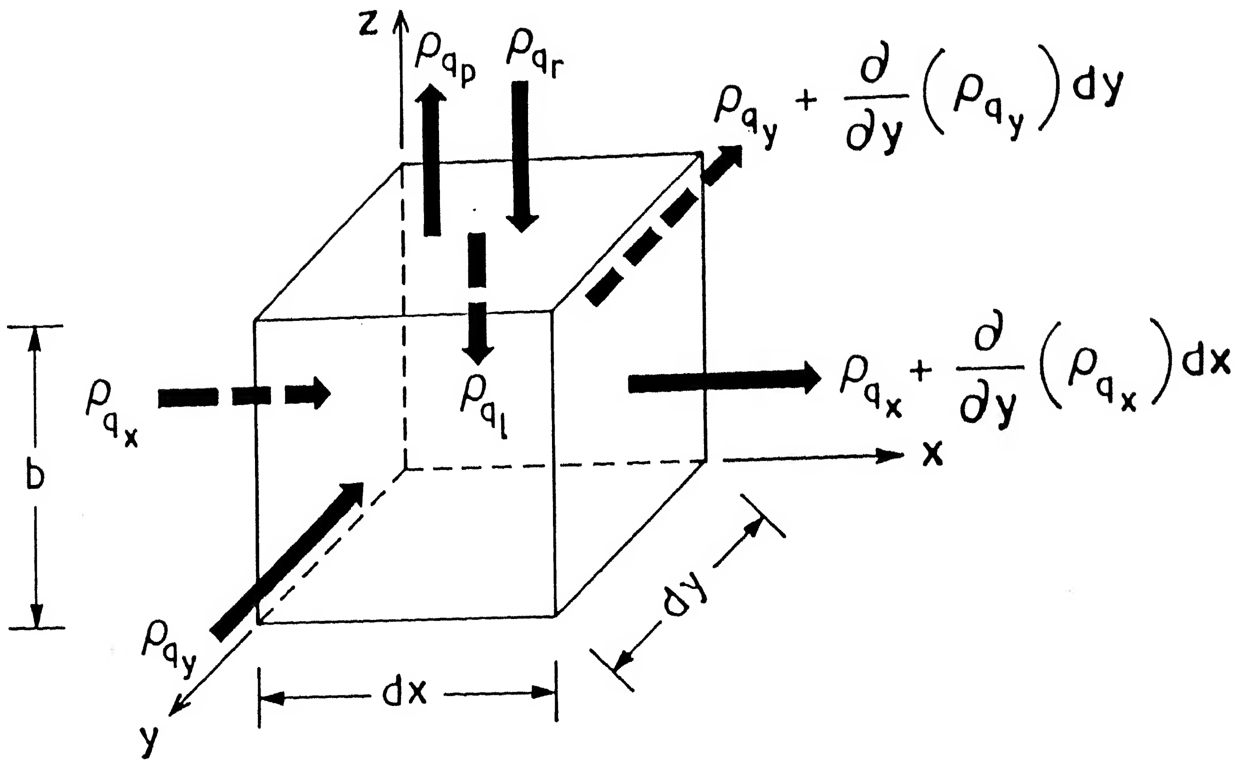


Fig. 3.3 Cartesian fixed control volume showing the influx and efflux of mass of water.

thickness of the confined aquifer. The fluxes of mass of water (kg/m^2 of porous medium/s) at each side of the control volume in two-dimensional flow is shown in Fig. 3.3. q_p, q_r and q_l represent respectively the specific distributed pumping (rate of artificial pumping per unit area), specific distributed recharge (rate of artificial recharge per unit area) and specific leakage (leakage rate per unit area through leaky aquifer). In case of point pumping and point recharge, q_p and q_r are expressed as:

$$q_p = \sum_{w \in \Omega_p} q_{pw} \, \delta(x-x_w, \, y-y_w) \tag{3.22}$$

$$q_r = \sum_{w \in \Omega_r} q_{rw} \, \delta(x-x_w, \, y-y_w) \tag{3.23}$$

Considering the mass of water as extensive property, the groundwater flow equation is obtained from the Reynolds transport theorem. Thus transient Groundwater Flow Equation (GFE) for two dimensional areal flow of a homogeneous compressible fluid through a heterogeneous anisotropic leaky confined aquifer system can be written as (Pinder and Bredehoeft, 1968; Freeze and Cherry, 1979; Konikow and Bredehoeft, 1984; Bear and Verruijt 1987, Willis and Yeh 1987):

$$\frac{\partial}{\partial x_i}\left(T_{ij} \frac{\partial h}{\partial x_j} \right) = S \frac{\partial h}{\partial t} + \sum_{w \in \Omega_p} q_{pw} \, \delta(x - x_w, \, y - y_w)$$

$$- \sum_{w \in \Omega_r} q_{rw} \, \delta(x - x_w, \, y - y_w) - \frac{K_{zz}^{ll}}{m} (h_s - h); \quad i, j = 1, 2 \tag{3.24}$$

Where

T_{ij} transmissivity tensor, $M^o L^2 T^{-1}$;

h hydraulic head, $M^o L T^o$;

x_i, x_j cartesian coordinates, $M^o L T^o$;

S storage coefficient, $M^o L^o T^o$;

t time, $M^o L^o T$;

q_{pw}, q_{rw} specific point pumping and recharge from the w^{th} pumping (or recharge) well located at (x_w, y_w) respectively, $M^o L T^{-1}$;

$\delta(x - x_w, y - y_w)$ Dirac delta function;

Ω_p, Ω_r index sets of the location of all pumping and recharge cells within the system respectively;

K^{ll}_{zz} vertical hydraulic conductivity of the leaky layer, $M^o L T^{-1}$;

m thickness of the leaky layer, $M^o L T^o$;

h_s hydraulic head in the source bed, $M^o L T^o$;

The Dirac delta function is defined as:

$$\delta(x - x_w, y - y_w) = \left| \begin{array}{l} 1, \text{ if } x = x_w, \ y = y_w \\ 0, \text{ if } x \neq x_w, \ y \neq y_w \end{array} \right. \tag{3.25}$$

Equation (3.24) describes the head distribution in the aquifer with respect to space and time, and is a linear partial differential equation.

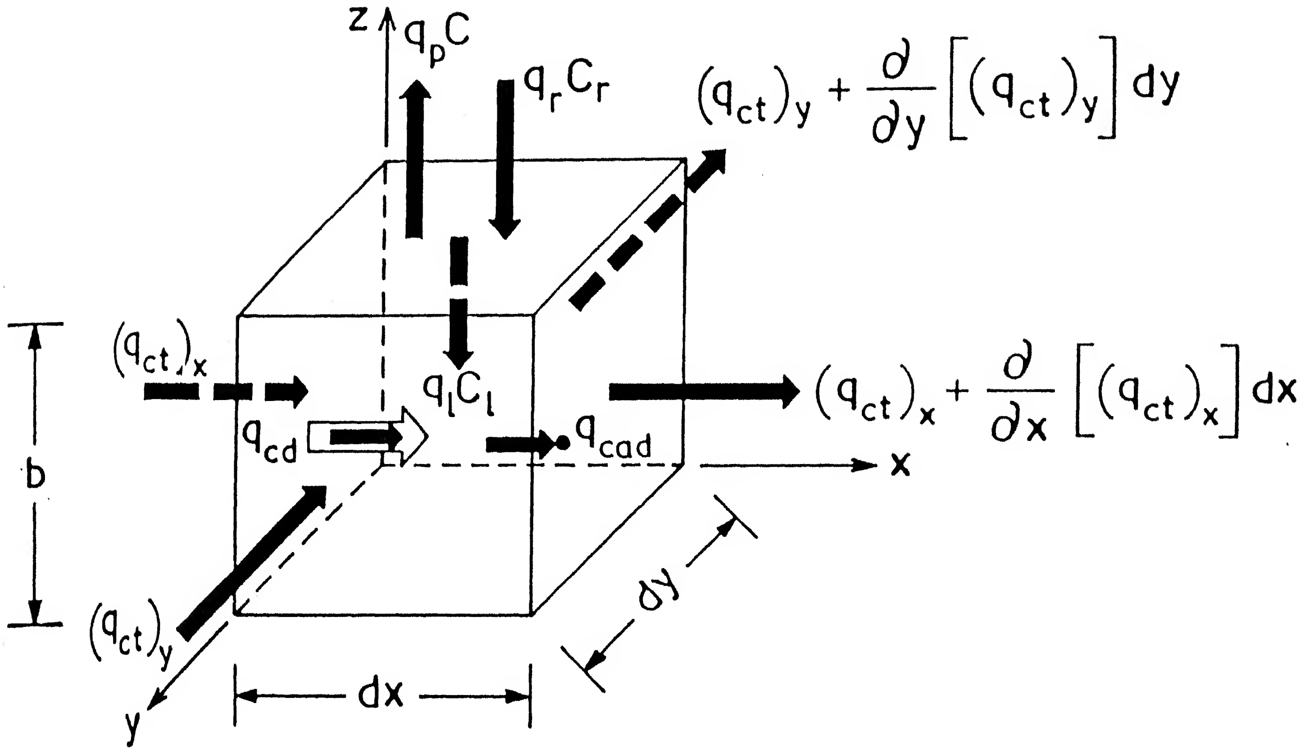


Fig. 3.4 Cartesian fixed control volume showing the influx and efflux of mass of pollutant.

1984; Bear and Verruijt, 1987):

$$R_d \frac{\partial}{\partial t}(b\ C) = \frac{\partial}{\partial x_i}\left[b\ (D_h)_{ij}\ \frac{\partial C}{\partial x_j}\right] - \frac{\partial}{\partial x_i}(b\ C\ v_i) - \lambda\ R_d\ b\ C$$

$$- \sum_{w \in \Omega_p} \frac{q_{pw}\ C}{n_{eff}}\ \delta(x - x_w,\ y - y_w) + \sum_{w \in \Omega_r} \frac{q_{rw}\ C_r}{n_{eff}}\ \delta(x - x_w,\ y - y_w)$$

$$+ K_{zz}^{ll}\ \frac{(h_s - h)\ C_l}{m\ n_{eff}} \quad ; \quad i,\ j = 1,\ 2 \qquad (3.28)$$

Where

R_d	retardation factor, $M^o\ L^o\ T^o$;
b	saturated aquifer thickness, $M^o\ L\ T^o$;
C	concentration of the dissolved chemical species, $M\ L^{-3}\ T^o$;
$(D_h)_{ij}$	hydrodynamic dispersion tensor, $M^o\ L^2\ T^{-1}$;
v_i	average seepage velocity in the direction i, $M^o\ L\ T^{-1}$;
λ	first order kinetic decay rate, $M^o\ L^o\ T^{-1}$;
n_{eff}	effective aquifer porosity, $M^o\ L^o\ T^o$;
C_r	solute concentration in recharge, $M\ L^{-3}\ T^o$;
C_l	solute concentration in leakage, $M\ L^{-3}\ T^o$;

Equation (3.28) describes the chemical concentration in the aquifer with respect to space and time, and is a nonlinear partial differential equation. The hydrodynamic dispersion tensor is defined as the sum of the mechanical dispersion and molecular diffusion

tensors:

$$(D_h)_{ij} = D_{ij} + (D_d^*)_{ij} \tag{3.29}$$

3.3.3 Dispersion coefficients

The mechanical dispersion coefficient depends upon the flow velocity, microscopic porous matrix configuration and molecular diffusion. Mathematically it can be expressed as (Bear, 1961; Scheidegger, 1961; Bear and Bachmet, 1967):

$$D_{ij} = a_{ijkm} \frac{v_k \, v_m}{|v|} f(P_e, l_r) \tag{3.30}$$

Where

a_{ijkm}	dispersivity of the aquifer, $M^o\ L\ T^o$;
v_k, v_m	velocity components in k and m directions respectively, $M^o\ L\ T^{-1}$;
$\|v\|$	magnitude of the velocity, $M^o\ L\ T^{-1}$;
P_e	Peclet number, $M^o\ L^o\ T^o$;
l_r	characteristic length ratio, $M^o\ L^o\ T^o$;

The characteristic length ratio is defined as the ratio of the length characterizing the individual pores of a porous medium to the length characterizing their cross-section. $f(P_e, l_r)$ is a function which introduces the effect of pollutant transfer by molecular diffusion between adjacent streamlines at the microscopic level. It

explains how the molecular diffusion is coupled with mechanical dispersion through Peclet number.

The coefficient a_{ijkm} is a fourth rank tensor which expresses the microscopic configuration of the solid-liquid interface. For an isotropic aquifer, this coefficient is defined in terms of longitudinal and transverse dispersivities of aquifer (α_L and α_T respectively, M^o L T^o). The expression for this dipersivity of the aquifer is given by (Bear, 1961; Scheidegger, 1961):

$$a_{ijkm} = \alpha_T \, \delta_{ij} \, \delta_{km} + \frac{\alpha_L - \alpha_T}{2} \left(\delta_{ik} \, \delta_{jm} + \delta_{im} \, \delta_{jk}\right) \tag{3.31}$$

Where δ_{ij} denotes the kronecker delta. The longitudinal and transverse dispersivities are related to the longitudinal and transverse dispersion coefficients (D_L and D_T respectively; M^o L^2 T^{-1}) by:

$$D_L = \alpha_L \, |v| \tag{3.32}$$

$$D_T = \alpha_T \, |v| \tag{3.33}$$

By combining Equations (3.30), (3.31), (3.32) and (3.33) and assuming $f(P_e, l_r) \approx 1$, the dispersion coefficient can be expressed as:

$$D_{ij} = D_T \, \delta_{ij} + (D_L - D_T) \frac{v_i \, v_j}{|v|^2} \tag{3.34}$$

In cartesian coordinates, for two-dimensional flow in an isotropic aquifer, the components of the dispersion coefficient can be stated explicitly as:

$$D_{xx} = D_L \left[\frac{v_x}{|v|} \right]^2 + D_T \left[\frac{v_y}{|v|} \right]^2 \qquad (3.35)$$

$$D_{yy} = D_T \left[\frac{v_x}{|v|} \right]^2 + D_L \left[\frac{v_y}{|v|} \right]^2 \qquad (3.36)$$

$$D_{xy} = D_{yx} = \left(D_L - D_T\right) \frac{v_x \, v_y}{|v|^2} \qquad (3.37)$$

From the Equations (3.35), (3.36) and (3.37), it is evident that D_{xx} and D_{yy} must have positive values, whereas D_{xy} may be negative depending upon the sign of v_x and v_y.

3.3.4 Assumptions

A number of assumptions have been made in the development of the groundwater flow equation, solute transport equation and dispersion coefficients. The main assumptions that must be carefully evaluated before applying the model to a field problem, are enumerated below:

1. Darcy's law is valid and hydraulic head gradients are the

only significant driving mechanism for fluid flow.

2. The flow in the confined aquifer is essentially horizontal, while it is vertical in the semipervious layer. This assumption remains valid when the hydraulic conductivity of the semipervious layer is at least one order less than that of confined aquifer.
3. The storage in the semipervious layer is ignored.
4. The porosity and hydraulic conductivity of the aquifer are constant with time, and porosity is uniform in space.
5. Gradients of fluid density, viscosity and temperature do not affect the velocity distribution.
6. No chemical reactions occur that affect the concentration of the solute, the fluid properties or the aquifer properties.
7. Ionic diffusion is negligible contributor to the total dispersive flux.
8. Vertical variations in head and concentration are negligible.
9. The aquifer is homogeneous and isotropic with respect to the coefficients of longitudinal and transverse dispersivity.

3.4 DISCRETIZATION OF FLOW AND TRANSPORT EQUATIONS

Finite difference and finite element methods are the most commonly used techniques to approximate the continuous partial differential equations as a set of discrete equations in time and space. For any given class of problems, the choice of the best

approach depends on the processes being modeled, the accuracy desired, and the effort that can be expended on obtaining a solution. The pros and cons associated with these two methods are briefly summarized in Table 3.2 (Pinder and Frind, 1972; Narasimhan and Witherspoon, 1976; Pinder and Gray, 1977; Mercer and Faust, 1981). These observations are based on: (a) ease in understanding the theoretical basis, (b) ease in programming, (c) ease in designing grid and preparing data input, (d) handling complex geometries, (e) approximation accuracy, (f) handling tensors, (g) handling low dispersion, and (h) solution efficiency. Discussion on various numerical methods available to approximate the partial differential equations encountered in subsurface simulation is available in Pinder (1988). For many groundwater applications, the subsurface boundaries are not that well known and thus difficulty in approximating a curved boundary using FDM is not a problem. The FDM is probably adequate for most groundwater flow problems.

The GFE and STE are discretized using the finite difference method in this thesis. The groundwater basin has been considered as a distributed parameter system. The area of interest of aquifer domain is subdivided by a grid system into a number of small sized subareas. The model developed here utilizes a rectangular, uniformly spaced, block-centered, finite-difference grid to approximate the groundwater flow and solute transport equations.

Table 3.2 Brief summary of important Advantages and disadvantages of FDM and FEM

Advantage	Disadvantage
FDM	
1. Intuitive basis	1. Law accurecy for some problems
2. Easy data input	2. Regular grids
3. Efficient matrix technique	3. Sharp fronts require special treatment
4. Ease in the modification of the program	
5. Error in the input of nodel locations doesn't arrise	
6. Generally require less CPU time	
FEM	
1. Flexible geometry	1. Mathematical basis is advanced
2. High accuracy easily included	2. Difficult data input
3. Evaluates cross product terms better	3. Difficult programming
4. For linear problems, sharp fronts can be tracked fairly accurately	4. Errors in the input of nodel locations in the Galerkin model can leed to computational problems that are difficult to detect
	5. For no n linear problems, tracking of sharp fronts may demonstrate numerical oscillation that becomes unstable
	6. Generally reqiure more CPU time

3.4.1 Discretization of groundwater flow equation

Fig. 3.5 shows a typical representation of node (i,j) associated with block-centered grid to discretize GFE. i and j indices are in the positive direction of x and negative direction of y respectively, while the index k (dimension for time, t) is pointing upward (in the positive direction of z) as shown in Fig. 3.5. Assuming the coordinates axes alined with the principal directions of the transmissivity vector, L.H.S. (Left Hand Side) of Equation (3.24) in cartesian coordinates can be written as:

$$\frac{\partial}{\partial x_i}\left[T_{ij}\frac{\partial h}{\partial x_j}\right] = \frac{\partial}{\partial x}\left[T_{xx}\frac{\partial h}{\partial x}\right] + \left[T_{yy}\frac{\partial h}{\partial y}\right] \qquad (3.38)$$

Using central difference for space derivative and taking arithmetic mean for the transmissivities,

$$\frac{\partial}{\partial x}\left[T_{xx}\frac{\partial h}{\partial x}\right] = \frac{1}{\Delta x}\left[\left(T_{xx}\frac{\partial h}{\partial x}\right)^k_{i+\frac{1}{2},j} - \left(T_{xx}\frac{\partial h}{\partial x}\right)^k_{i-\frac{1}{2},j}\right]$$

$$= \frac{1}{\Delta x}\left[\left(T_{xx}\right)_{i+\frac{1}{2},j}\left\{\frac{h^k_{i+1,j} - h^k_{i,j}}{\Delta x}\right\} - \left(T_{xx}\right)_{i-\frac{1}{2},j}\left\{\frac{h^k_{i,j} - h^k_{i-1,j}}{\Delta x}\right\}\right]$$

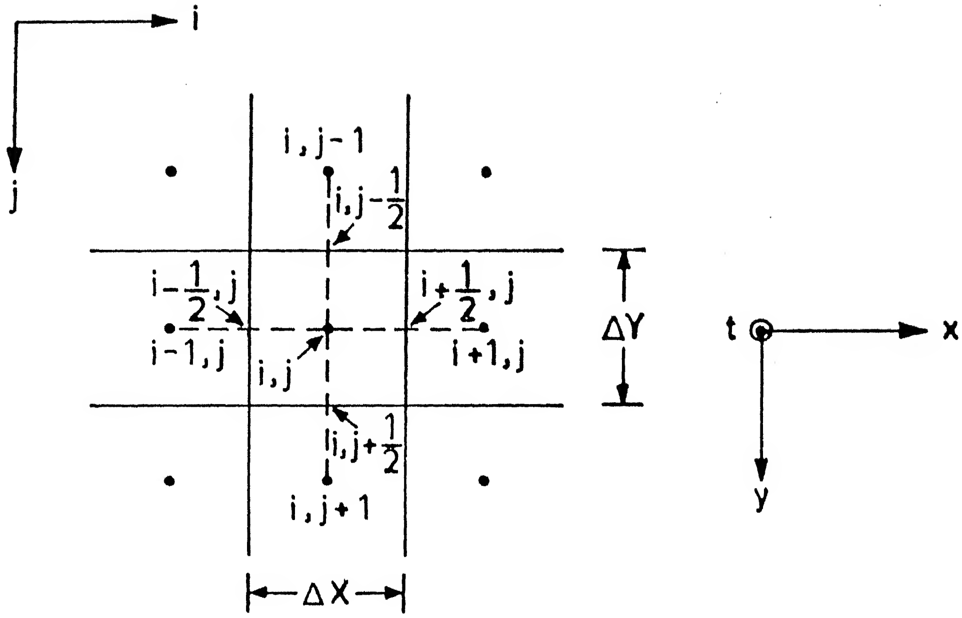


Fig. 3.5 Typical representation of node (i, j) associated with block-centered grid to discretize GFE.

$$= \frac{1}{2\,\Delta x^2}\left[\left(T_{xx}\right)_{i+1,j} + \left(T_{xx}\right)_{i,j}\right]\left[h^k_{i+1,j} - h^k_{i,j}\right]$$

$$- \frac{1}{2\,\Delta x^2}\left[\left(T_{xx}\right)_{i,j} + \left(T_{xx}\right)_{i-1,j}\right]\left[h^k_{i,j} - h^k_{i-1,j}\right]$$

(3.39)

and

$$\frac{\partial}{\partial y}\left[T_{yy}\frac{\partial h}{\partial y}\right] = \frac{1}{\Delta y}\left[\left(T_{yy}\frac{\partial h}{\partial y}\right)^k_{i,j+\frac{1}{2}} - \left(T_{yy}\frac{\partial h}{\partial y}\right)^k_{i,j-\frac{1}{2}}\right]$$

$$= \frac{1}{\Delta y}\left[\left(T_{yy}\right)_{i,j+\frac{1}{2}}\left\{\frac{h^k_{i,j+1} - h^k_{i,j}}{\Delta y}\right\} - \left(T_{yy}\right)_{i,j-\frac{1}{2}}\left\{\frac{h^k_{i,j} - h^k_{i,j-1}}{\Delta y}\right\}\right]$$

$$= \frac{1}{2\,\Delta y^2}\left[\left(T_{yy}\right)_{i,j+1} + \left(T_{yy}\right)_{i,j}\right]\left[h^k_{i,j+1} - h^k_{i,j}\right]$$

$$- \frac{1}{2\,\Delta y^2}\left[\left(T_{yy}\right)_{i,j} + \left(T_{yy}\right)_{i,j-1}\right]\left[h^k_{i,j} - h^k_{i,j-1}\right]$$

(3.40)

Where

$$(T_{xx})_{i+\frac{1}{2},j} = \frac{(T_{xx})_{i+1,j} + (T_{xx})_{i,j}}{2} \qquad (3.41)$$

$$(T_{xx})_{i-\frac{1}{2},j} = \frac{(T_{xx})_{i,j} + (T_{xx})_{i-1,j}}{2} \tag{3.42}$$

$$(T_{yy})_{i,j+\frac{1}{2}} = \frac{(T_{yy})_{i,j+1} + (T_{yy})_{i,j}}{2} \tag{3.43}$$

$$(T_{yy})_{i,j-\frac{1}{2}} = \frac{(T_{yy})_{i,j} + (T_{yy})_{i,j-1}}{2} \tag{3.44}$$

Using backward difference for time derivative,

$$S \frac{\partial h}{\partial t} = S_{i,j} \frac{h^{k}_{i,j} - h^{k-1}_{i,j}}{\Delta t} \tag{3.45}$$

Thus, Equation (3.24) in the implicit form can be approximated as:

$$(FC_2)_{i,j}\, h^{k}_{i,j-1} + (FC_3)_{i,j}\, h^{k}_{i+1,j} + (FC_4)_{i,j}\, h^{k}_{i,j+1}$$

$$+ (FC_5)_{i,j}\, h^{k}_{i-1,j} + (FC_6)^{k}_{i,j} - (FC_1)^{k}_{i,j}\, h^{k}_{i,j} = 0 \tag{3.46}$$

Where FC_1, FC_2, FC_3, FC_4, FC_5 and FC_6 are Flow Coefficients (FC), and indices i, j and k represent x, y and t dimensions respectively. The flow coefficients FC_1, FC_2, FC_3, FC_4 and FC_5 depend upon the system parameters only. The flow coefficient FC_6 depends on the

system parameters as well as hydraulic stresses such as pumping and recharge, and hydrodynamic strengths such as hydraulic head. Mathematically FC can be expressed as:

$$FC = f(T_{xx}, T_{yy}, S, K_{zz}^{11}, \Delta x, \Delta y, \Delta t, m, h_s, h, Q_p, Q_r) \qquad (3.47)$$

Where T_{xx} and T_{yy} denote principal transmissivities in x and y directions respectively. Q_p and Q_r denote pumping and recharge (M^o L^3 T^{-1}) respectively, and f(.) denotes a function of given arguments. These coefficients are given by:

$$FC_1 = \frac{1}{2\,\Delta x^2}\left[(T_{xx})_{i-1,j} + 2\,(T_{xx})_{i,j} + (T_{xx})_{i+1,j}\right]$$

$$+ \frac{1}{2\,\Delta y^2}\left[(T_{yy})_{i,j-1} + 2\,(T_{yy})_{i,j} + (T_{yy})_{i,j+1}\right]$$

$$+ \frac{S_{i,j}}{\Delta t} + \frac{K_{zz}^{11}}{m_{i,j}^{k}} \qquad (3.48)$$

$$FC_2 = \frac{(T_{yy})_{i,j-1} + (T_{yy})_{i,j}}{2\,\Delta y^2} \qquad (3.49)$$

$$FC_3 = \frac{(T_{xx})_{i+1,j} + (T_{xx})_{i,j}}{2\,\Delta x^2} \qquad (3.50)$$

$$FC_4 = \frac{(T_{yy})_{i,j+1} + (T_{yy})_{i,j}}{2\ \Delta y^2} \tag{3.51}$$

$$FC_5 = \frac{(T_{xx})_{i-1,j} + (T_{xx})_{i,j}}{2\ \Delta x^2} \tag{3.52}$$

$$FC_6 = \frac{S_{i,j}\ h^{k-1}_{i,j}}{\Delta t} - \frac{(Q_p)^k_{i,j}\ (\delta_p)_{i,j}}{\Delta x\ \Delta y} + \frac{(Q_r)^k_{i,j}\ (\delta_r)_{i,j}}{\Delta x\ \Delta y}$$

$$+ \frac{(K^{11}_{zz})_{i,j}\ (h_s)^k_{i,j}}{m^k_{i,j}} \tag{3.53}$$

Where $(\delta_p)_{i,j}$ and $(\delta_r)_{i,j}$ represent the magnitudes of Dirac delta function for the pumping and recharge at node (i,j) respectively.

3.4.2 Discretization of solute transport equation

The first and second terms of R.H.S. (Right Hand Side) of Equation (3.28) in cartesian coordinates can be written as:

$$\frac{\partial}{\partial x_i}\left[b\ (D_h)_{ij}\ \frac{\partial C}{\partial x_j}\right] = \frac{\partial}{\partial x}\left[b\ D_{hxx}\ \frac{\partial C}{\partial x} + b\ D_{hxy}\ \frac{\partial C}{\partial y}\right]$$

$$+ \frac{\partial}{\partial y}\left[b\ D_{hyx}\ \frac{\partial C}{\partial x} + b\ D_{hyy}\ \frac{\partial C}{\partial y}\right] \tag{3.54}$$

and

$$\frac{\partial}{\partial x_i}\left(b\ C\ v_i\right) = v_i\left[C\ \frac{\partial b}{\partial x_i} + b\ \frac{\partial C}{\partial x_i}\right] + b\ C\ \frac{\partial v_i}{\partial x_i}$$

$$= b\ v_i\ \frac{\partial C}{\partial x_i} + C\ \frac{\partial}{\partial x_i}(b\ v_i) \tag{3.55}$$

Using Darcy's law, Equation (3.55) can be written as:

$$\frac{\partial}{\partial x_i}\left(b\ C\ v_i\right) = b\ v_i\ \frac{\partial C}{\partial x_i} - \frac{C}{n_{eff}}\ \frac{\partial}{\partial x_i}\left(T_{ij}\ \frac{\partial h}{\partial x_j}\right) \tag{3.56}$$

Using Groundwater Flow Equation, Equation (3.56) can be written as:

$$\frac{\partial}{\partial x_i}\left(b\ C\ v_i\right) = b\ v_x\ \frac{\partial C}{\partial x} + b\ v_y\ \frac{\partial C}{\partial y} - \frac{C}{n_{eff}}\left[S\ \frac{\partial h}{\partial t} + q_p\ \delta_p - q_r\ \delta_r - q_l\right] \tag{3.57}$$

Where q_p, q_r and q_l represent specific point pumping, specific point recharge and leakage respectively. δ_p and δ_r denote the magnitudes of Dirac delta function for the specific point pumping and specific point recharge respectively. The specific leakage through the leaky layer is expresses as:

$$q_l = \frac{K^{ll}_{zz}}{m}\left(h_s - h\right) \tag{3.58}$$

Assuming retardation factor equal to one, the L.H.S. of

Equation (3.28) can be written as:

$$\frac{\partial}{\partial t}(b\ C) = \left[b\ \frac{\partial C}{\partial t} + C\ \frac{\partial b}{\partial t}\right] \tag{3.59}$$

Thus, Equation (3.28) in cartesian coordinates can be written as:

$$b\ \frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left[b\ D_{hxx}\ \frac{\partial C}{\partial x} + b\ D_{hxy}\ \frac{\partial C}{\partial y}\right] + \frac{\partial}{\partial y}\left[b\ D_{hyx}\ \frac{\partial C}{\partial x} + b\ D_{hyy}\ \frac{\partial C}{\partial y}\right] - v_x\ b\ \frac{\partial C}{\partial x} - v_y\ b\ \frac{\partial C}{\partial y} + \frac{C}{n_{eff}}\ S\ \frac{\partial h}{\partial t}$$

$$- \frac{q_r\ \delta_r}{n_{eff}}\left(C - C_r\right) - \frac{q_1}{n_{eff}}\left(C - C_1\right) - \lambda\ b\ C - C\ \frac{\partial b}{\partial t} \tag{3.60}$$

$$= I^{st} + II^{nd} + III^{rd} + IV^{th} + V^{th} + VI^{th} + VII^{th}$$

$$+ VIII^{th} + IX^{th}$$

(9 components)

Fig 3.6 shows a typical representation of node (i,j) associated with block-centered grid to discretize the STE. Again, i and j indices are in the positive direction of x and negative direction of y respectively, while the index k is pointing upward (in the positive direction of z) as shown in Fig. 3.6.

Using central difference for space derivatives and backward difference for time derivative, the nine components of R.H.S. and

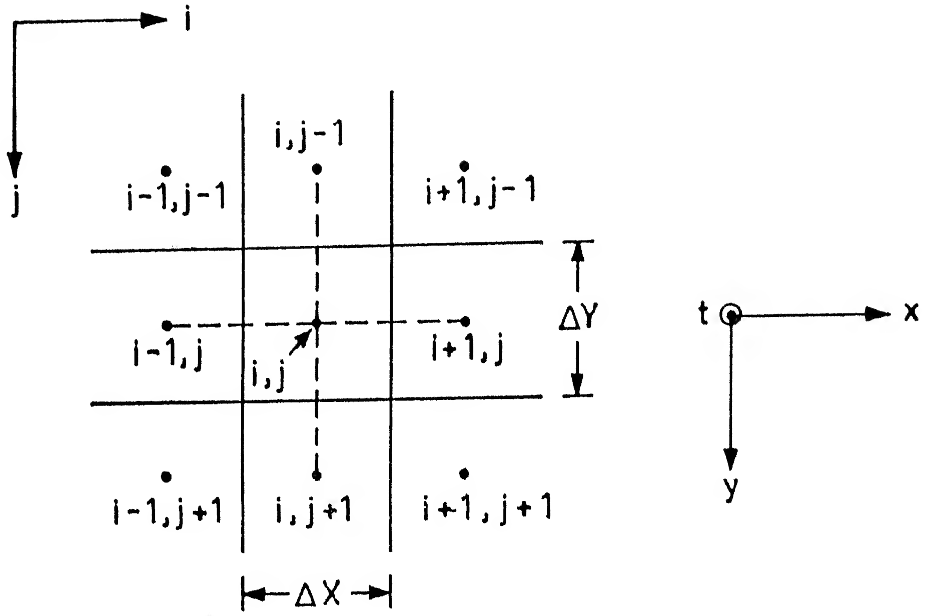


Fig. 3.6 Typical representation of node (i,j) associated with block-centered grid to discretize STE.

L.H.S. of Equation (3.60) can be approximated as:

$$I^{st} \text{ component} = \frac{\left[b\ D_{hxx} \frac{\partial C}{\partial x}\right]^k_{i+\frac{1}{2},j} - \left[b\ D_{hxx} \frac{\partial C}{\partial x}\right]^k_{i-\frac{1}{2},j}}{\Delta x}$$

$$+ \frac{\left[b\ D_{hxy} \frac{\partial C}{\partial y}\right]^k_{i+\frac{1}{2},j} - \left[b\ D_{hxy} \frac{\partial C}{\partial y}\right]^k_{i-\frac{1}{2},j}}{\Delta x} \quad (3.61)$$

The concentration gradients are evaluated as:

$$\left(\frac{\partial C}{\partial x}\right)^k_{i+\frac{1}{2},j} = \frac{C^k_{i+1,j} - C^k_{i,j}}{\Delta x} \quad (3.62)$$

$$\left(\frac{\partial C}{\partial x}\right)^k_{i-\frac{1}{2},j} = \frac{C^k_{i,j} - C^k_{i-1,j}}{\Delta x} \quad (3.63)$$

$$\left(\frac{\partial C}{\partial y}\right)^k_{i+\frac{1}{2},j} = \frac{C^k_{i+\frac{1}{2},j+1} - C^k_{i+\frac{1}{2},j-1}}{2\ \Delta y} \quad (3.64)$$

$$\left(\frac{\partial C}{\partial y}\right)^k_{i-\frac{1}{2},j} = \frac{C^k_{i-\frac{1}{2},j+1} - C^k_{i-\frac{1}{2},j-1}}{2\ \Delta y} \quad (3.65)$$

Where

$$C^k_{i+\frac{1}{2},j+1} = \frac{C^k_{i+1,j+1} + C^k_{i,j+1}}{2} \quad (3.66)$$

$$c^k_{i+\frac{1}{2},j-1} = \frac{c^k_{i,j-1} + c^k_{i+1,j-1}}{2} \qquad (3.67)$$

$$c^k_{i-\frac{1}{2},j+1} = \frac{c^k_{i-1,j+1} + c^k_{i,j+1}}{2} \qquad (3.68)$$

$$c^k_{i-\frac{1}{2},j-1} = \frac{c^k_{i-1,j-1} + c^k_{i,j-1}}{2} \qquad (3.69)$$

Thus, Equation (3.61) can be written as:

$$
\begin{aligned}
I^{st} \text{ component} = {} & \frac{\left[b\ D_{hxx}\right]^k_{i+\frac{1}{2},j} \left(c^k_{i+1,j} - c^k_{i,j}\right)}{\Delta x^2} \\
& - \frac{\left[b\ D_{hxx}\right]^k_{i-\frac{1}{2},j} \left(c^k_{i,j} - c^k_{i-1,j}\right)}{\Delta x^2} \\
& + \frac{\left[b\ D_{hxy}\right]^k_{i+\frac{1}{2},j} \left(c^k_{i,j+1} + c^k_{i+1,j+1} - c^k_{i,j-1} - c^k_{i+1,j-1}\right)}{4\ \Delta x\ \Delta y} \\
& - \frac{\left[b\ D_{hxy}\right]^k_{i-\frac{1}{2},j} \left(c^k_{i-1,j+1} + c^k_{i,j+1} - c^k_{i-1,j-1} - c^k_{i,j-1}\right)}{4\ \Delta x\ \Delta y}
\end{aligned}
\qquad (3.70)
$$

$$\mathrm{II}^{nd}\ \text{component} = \frac{\left[b\ D_{hyx}\ \frac{\partial C}{\partial x}\right]^{k}_{i,j+\frac{1}{2}} - \left[b\ D_{hyx}\ \frac{\partial C}{\partial x}\right]^{K}_{i,j-\frac{1}{2}}}{\Delta y}$$

$$+ \frac{\left[b\ D_{hyy}\ \frac{\partial C}{\partial y}\right]^{k}_{i,j+\frac{1}{2}} - \left[b\ D_{hyy}\ \frac{\partial C}{\partial y}\right]^{k}_{i,j-\frac{1}{2}}}{\Delta y} \tag{3.71}$$

The concentration gradients are evaluated as:

$$\left(\frac{\partial C}{\partial x}\right)^{k}_{i,j+\frac{1}{2}} = \frac{C^{k}_{i+1,j+\frac{1}{2}} - C^{k}_{i-1,j+\frac{1}{2}}}{2\ \Delta x} \tag{3.72}$$

$$\left(\frac{\partial C}{\partial x}\right)^{k}_{i,j-\frac{1}{2}} = \frac{C^{k}_{i+1,j-\frac{1}{2}} - C^{k}_{i-1,j-\frac{1}{2}}}{2\ \Delta x} \tag{3.73}$$

$$\left(\frac{\partial C}{\partial y}\right)^{k}_{i,j+\frac{1}{2}} = \frac{C^{k}_{i,j+1} - C^{k}_{i,j}}{\Delta y} \tag{3.74}$$

$$\left(\frac{\partial C}{\partial y}\right)^{k}_{i,j-\frac{1}{2}} = \frac{C^{k}_{i,j} - C^{k}_{i,j-1}}{\Delta y} \tag{3.75}$$

Where

$$C^{k}_{i+1,j+\frac{1}{2}} = \frac{C^{k}_{i+1,j} + C^{k}_{i+1,j+1}}{2} \tag{3.76}$$

$$c^k_{i-1,j+\frac{1}{2}} = \frac{c^k_{i-1,j} + c^k_{i-1,j+1}}{2} \tag{3.77}$$

$$c^k_{i+1,j-\frac{1}{2}} = \frac{c^k_{i+1,j-1} + c^k_{i+1,j}}{2} \tag{3.78}$$

$$c^k_{i-1,j-\frac{1}{2}} = \frac{c^k_{i-1,j-1} + c^k_{i-1,j}}{2} \tag{3.79}$$

Thus, Equation (3.71) can be written as:

II^{nd} component =

$$\frac{\left[b\ D_{hyx}\right]^k_{i,j+\frac{1}{2}} \left(c^k_{i+1,j} + c^k_{i+1,j+1} - c^k_{i-1,j} - c^k_{i-1,j+1}\right)}{4\ \Delta x\ \Delta y}$$

$$- \frac{\left[b\ D_{hyx}\right]^k_{i,j-\frac{1}{2}} \left(c^k_{i+1,j-1} + c^k_{i+1,j} - c^k_{i-1,j-1} - c^k_{i-1,j}\right)}{4\ \Delta x\ \Delta y}$$

$$+ \frac{\left[b\ D_{hyy}\right]^k_{i,j+\frac{1}{2}} \left(c^k_{i,j+1} - c^k_{i,j}\right)}{\Delta y^2}$$

$$- \frac{\left[b\ D_{hyy}\right]^k_{i,j-\frac{1}{2}} \left(c^k_{i,j} - c^k_{i,j-1}\right)}{\Delta y^2} \tag{3.80}$$

$$\text{III}^{rd} \quad \text{component} = - (v_x)^k_{i,j}\, b^k_{i,j} \frac{c^k_{i+1,j} - c^k_{i-1,j}}{2\,\Delta x} \tag{3.81}$$

$$\text{IV}^{th} \quad \text{component} = - (v_y)^k_{i,j}\, b^k_{i,j} \frac{c^k_{i,j+1} - c^k_{i,j-1}}{2\,\Delta y} \tag{3.82}$$

$$\text{V}^{th} \quad \text{component} = \frac{c^k_{i,j}}{n_{eff}}\, S_{i,j} \frac{\left(h^k_{i,j} - h^{k-1}_{i,j}\right)}{\Delta t} \tag{3.83}$$

$$\text{VI}^{th} \quad \text{component} = - \frac{(Q_r)^k_{i,j}\, (\delta_r)_{i,j} \left(c^k_{i,j} - (c_r)^k_{i,j}\right)}{n_{eff}\, \Delta x\, \Delta y} \tag{3.84}$$

$$\text{VII}^{th} \quad \text{component} = - \frac{(K^{ll}_{zz})_{i,j}}{m^k_{i,j}\, n_{eff}} \left((h_s)^k_{i,j} - h^k_{i,j}\right)\left(c^k_{i,j} - (c_l)^k_{i,j}\right) \tag{3.85}$$

$$\text{VIII}^{th} \quad \text{component} = - \lambda\, b^k_{i,j}\, c^k_{i,j} \tag{3.86}$$

$$\text{IX}^{th} \quad \text{component} = - \frac{(c^k_{i,j})\,(b^k_{i,j} - b^{k-1}_{i,j})}{\Delta t} \tag{3.87}$$

Finally the implicit finite difference form of Equation (3.60) can

be written as:

$$(TC_2)^k_{i,j}\, C^k_{i-1,j-1} + (TC_3)^k_{i,j}\, C^k_{i,j-1} + (TC_4)^k_{i,j}\, C^k_{i+1,j-1}$$

$$+ (TC_5)^k_{i,j}\, C^k_{i+1,j} + (TC_6)^k_{i,j}\, C^k_{i+1,j+1} + (TC_7)^k_{i,j}\, C^k_{i,j+1}$$

$$+ (TC_8)^k_{i,j}\, C^k_{i-1,j+1} + (TC_9)^k_{i,j}\, C^k_{i-1,j} + (TC_{10})^k_{i,j}$$

$$- (TC_1)^k_{i,j}\, C^k_{i,j} = 0 \tag{3.88}$$

Where TC_1, TC_2, TC_3, TC_4, TC_5, TC_6, TC_7, TC_8, TC_9 and TC_{10} are Transport Coefficients (TC). The transport coefficients are the functions of system parameters, hydraulic stresses such as pumping and recharge, and hydrodynamic strengths such as hydraulic head and concentration of pollutant. Mathematically it can be expressed as:

$$TC = f(D_{hxx}, D_{hyy}, D_{hxy}, \Delta x, \Delta y, \Delta t, S, n_{eff}, h, K^{11}_{zz}, m, h_s, \lambda,$$
$$b, Q_r, K_{xx}, K_{yy}, C_r, C_1, C, R_d) \tag{3.89}$$

These transport coefficients for the nonsorble substance are expressed as:

$$TC_1 = \frac{\left(b\ D_{hxx} \right)^k_{i+\frac{1}{2},j}}{\Delta x^2} + \frac{\left(b\ D_{hxx} \right)^k_{i-\frac{1}{2},j}}{\Delta x^2} + \frac{\left(b\ D_{hyy} \right)^k_{i,j+\frac{1}{2}}}{\Delta y^2}$$

$$+ \frac{\left(b\ D_{hyy} \right)^k_{i,j-\frac{1}{2}}}{\Delta y^2} - \frac{S_{i,j} \left(h^k_{i,j} - h^{k-1}_{i,j} \right)}{n_{eff}\ \Delta t} + \frac{(Q_r)^k_{i,j}\ (\delta_r)_{i,j}}{n_{eff}\ \Delta x\ \Delta y}$$

$$+ \frac{\left(K^{11}_{zz} \right)_{i,j}}{m^k_{i,j}\ n_{eff}} \left[(h_s)^k_{i,j} - h^k_{i,j} \right] + \lambda\ b^k_{i,j} + \frac{b^k_{i,j} - b^{k-1}_{i,j}}{\Delta t}$$

$$+ \frac{b^k_{i,j}}{\Delta t} \tag{3.90}$$

$$TC_2 = \frac{1}{4\ \Delta x\ \Delta y} \left[\left(b\ D_{hxy} \right)^k_{i-\frac{1}{2},j} + \left(b\ D_{hyx} \right)^k_{i,j-\frac{1}{2}} \right] \tag{3.91}$$

$$TC_3 = \frac{\left(b\ D_{hyy} \right)^k_{i,j-\frac{1}{2}}}{\Delta y^2} + \frac{\left(b\ D_{hxy} \right)^k_{i-\frac{1}{2},j}}{4\ \Delta x\ \Delta y} - \frac{\left(b\ D_{hxy} \right)^k_{i+\frac{1}{2},j}}{4\ \Delta x\ \Delta y}$$

$$+ \frac{(v_y)^k_{i,j}\ b^k_{i,j}}{2\ \Delta y} \tag{3.92}$$

$$TC_4 = \frac{1}{4\ \Delta x\ \Delta y} \left[-\left(b\ D_{hxy} \right)^k_{i+\frac{1}{2},j} - \left(b\ D_{hyx} \right)^k_{i,j-\frac{1}{2}} \right] \qquad (3.93$$

$$TC_5 = \frac{\left[b\ D_{hxx} \right]^k_{i+\frac{1}{2},j}}{\Delta x^2} + \frac{\left[b\ D_{hyx} \right]^k_{i,j+\frac{1}{2}}}{4\ \Delta x\ \Delta y} - \frac{\left[b\ D_{hyx} \right]^k_{i,j-\frac{1}{2}}}{4\ \Delta x\ \Delta y}$$

$$- \frac{(v_x)^k_{i,j}\ b^k_{i,j}}{2\ \Delta x} \tag{3.94}$$

$$TC_6 = \frac{1}{4\ \Delta x\ \Delta y}\left[\left(b\ D_{hxy} \right)^k_{i+\frac{1}{2},j} + \left(b\ D_{hyx} \right)^k_{i,j+\frac{1}{2}} \right] \tag{3.95}$$

$$TC_7 = \frac{\left[b\ D_{hyy} \right]^k_{i,j+\frac{1}{2}}}{\Delta y^2} - \frac{\left[b\ D_{hxy} \right]^k_{i-\frac{1}{2},j}}{4\ \Delta x\ \Delta y} + \frac{\left[b\ D_{hxy} \right]^k_{i+\frac{1}{2},j}}{4\ \Delta x\ \Delta y}$$

$$- \frac{(v_y)^k_{i,j}\ b^k_{i,j}}{2\ \Delta y} \tag{3.96}$$

$$TC_8 = \frac{1}{4\ \Delta x\ \Delta y}\left[-\left(b\ D_{hxy} \right)^k_{i-\frac{1}{2},j} - \left(b\ D_{hyx} \right)^k_{i,j+\frac{1}{2}} \right] \tag{3.97}$$

$$TC_9 = \frac{\left[b\ D_{hxx} \right]^k_{i-\frac{1}{2},j}}{\Delta x^2} + \frac{\left[b\ D_{hyx} \right]^k_{i,j-\frac{1}{2}}}{4\ \Delta x\ \Delta y} - \frac{\left[b\ D_{hyx} \right]^k_{i,j+\frac{1}{2}}}{4\ \Delta x\ \Delta y}$$

$$+ \frac{(v_x)^k_{i,j}\ b^k_{i,j}}{2\ \Delta x} \tag{3.98}$$

$$TC_{10} = \frac{(Q_r)^k_{i,j}\ (C_r)^k_{i,j}\ (\delta_r)_{i,j}}{n_{eff}\ \Delta x\ \Delta y}$$

$$+ \frac{(K^{11}_{zz})_{i,j}}{m^k_{i,j}\ n_{eff}} \left[(h_s)^k_{i,j} - h^k_{i,j} \right] (C_1)^k_{i,j} + \frac{b^k_{i,j}\ C^{k-1}_{i,j}}{\Delta t} \tag{3.99}$$

3.4.2.1 Computation of velocity components

The velocity components present in the transport coefficients are computed using Darcy's law as discussed in section 3.2.1. Thus, these components are expresses as:

$$(v_x)^k_{i,j} = - \frac{(K_{xx})_{i,j} \left(h^k_{i+1,j} - h^k_{i-1,j}\right)}{2\ n_{eff}\ \Delta x} \tag{3.100}$$

$$(v_y)^k_{i,j} = - \frac{(K_{yy})_{i,j} \left(h^k_{i,j+1} - h^k_{i,j-1}\right)}{2\ n_{eff}\ \Delta y} \tag{3.101}$$

3.4.2.2 Computation of dispersion coefficients

However, the solute transport equation is discretized for the two-dimensional advective-dispersive-diffusive transport with linear decay in a two-dimensional flow environment for a leaky confined aquifer. The application of the model is illustrated for the cases having negligible diffusion contribution. It is because, for most situations, the contribution of molecular diffusion to hydrodynamic

dispersion is negligible when compared to convective diffusion (Marino, 1981). In such cases, the hydrodynamic dispersion tensor can be approximately taken equal to mechanical dispersion tensor:

$$(D_h)_{ij} \approx D_{ij} \tag{3.102}$$

Thus, dispersion coefficients at cell boundaries are computed from the following expressions:

$$\left(D_{xx} \right)^k_{i+\frac{1}{2},j} = \left(D_L \right)^k_{i+\frac{1}{2},j} \frac{\left[\left(v_x \right)^k_{i+\frac{1}{2},j} \right]^2}{\left[v^k_{i+\frac{1}{2},j} \right]^2} + \left(D_T \right)^k_{i+\frac{1}{2},j} \frac{\left[\left(v_y \right)^k_{i+\frac{1}{2},j} \right]^2}{\left[v^k_{i+\frac{1}{2},j} \right]^2} \tag{3.103}$$

$$\left(D_{yy} \right)^k_{i,j+\frac{1}{2}} = \left(D_L \right)^k_{i,j+\frac{1}{2}} \frac{\left[\left(v_y \right)^k_{i,j+\frac{1}{2}} \right]^2}{\left[v^k_{i,j+\frac{1}{2}} \right]^2} + \left(D_T \right)^k_{i,j+\frac{1}{2}} \frac{\left[\left(v_x \right)^k_{i,j+\frac{1}{2}} \right]^2}{\left[v^k_{i,j+\frac{1}{2}} \right]^2} \tag{3.104}$$

$$\left(D_{xy} \right)^k_{i+\frac{1}{2},j} = \left[\left(D_L \right)^k_{i+\frac{1}{2},j} - \left(D_T \right)^k_{i+\frac{1}{2},j} \right] \frac{(v_x)^k_{i+\frac{1}{2},j} \, (v_y)^k_{i+\frac{1}{2},j}}{\left[v^k_{i+\frac{1}{2},j} \right]^2} \tag{3.105}$$

$$\left(D_{yx} \right)^{k}_{i,j+\frac{1}{2}} = \left[\left(D_L \right)^{k}_{i,j+\frac{1}{2}} - \left(D_T \right)^{k}_{i,j+\frac{1}{2}} \right] \frac{(v_x)^{k}_{i,j+\frac{1}{2}} \, (v_y)^{k}_{i,j+\frac{1}{2}}}{\left[v^{k}_{i,j+\frac{1}{2}} \right]^2} \tag{3.106}$$

Where

$$(D_L)^{k}_{i+\frac{1}{2},j} = \alpha_L \; v^{k}_{i+\frac{1}{2},j} \tag{3.107}$$

$$(D_T)^{k}_{i+\frac{1}{2},j} = \alpha_T \; v^{k}_{i+\frac{1}{2},j} \tag{3.108}$$

$$(D_L)^{k}_{i,j+\frac{1}{2}} = \alpha_L \; v^{k}_{i,j+\frac{1}{2}} \tag{3.109}$$

$$(D_T)^{k}_{i,j+\frac{1}{2}} = \alpha_T \; v^{k}_{i,j+\frac{1}{2}} \tag{3.110}$$

The velocities are computed from the following expressions:

$$(v_x)^{k}_{i+\frac{1}{2},j} = - \frac{(K_{xx})_{i+1,j} + (K_{xx})_{i,j}}{2 \; n_{eff}} \; \frac{h^{k}_{i+1,j} - h^{k}_{i,j}}{\Delta x} \tag{3.111}$$

$$(v_y)^{k}_{i,j+\frac{1}{2}} = - \frac{(K_{yy})_{i,j+1} + (K_{yy})_{i,j}}{2 \; n_{eff}} \; \frac{h^{k}_{i,j+1} - h^{k}_{i,j}}{\Delta y} \tag{3.112}$$

$$(v_x)^{k}_{i,j+\frac{1}{2}} = \frac{1}{4} \left[(v_x)^{k}_{i-\frac{1}{2},j} + (v_x)^{k}_{i+\frac{1}{2},j} + (v_x)^{k}_{i-\frac{1}{2},j+1} + (v_x)^{k}_{i+\frac{1}{2},j+1} \right] \tag{3.113}$$

$$(v_y)^k_{i+\frac{1}{2},j} = \frac{1}{4}\left[(v_y)^k_{i,j-\frac{1}{2}} + (v_y)^k_{i+1,j-\frac{1}{2}} + (v_y)^k_{i+1,j+\frac{1}{2}} + (v_y)^k_{i,j+\frac{1}{2}}\right] \tag{3.114}$$

Equations (3.46) and (3.88) represent the finite difference forms of the flow and transport equations respectively. These discretized equations are embedded as equality constraints within the optimization model.

3.5 INTEGRATED MANAGEMENT MODEL

The management model for regional groundwater system should incorporate both quality and quantity aspects together. This integrated aquifer management is attracting greater attention because of substantial increase in the degradation of groundwater quality. The integrated management model can be described as a blend of groundwater simulation and optimization methods, because the equations governing the physical and chemical processes are embedded as constraints in the optimization model. Thus, the proposed integrated management model can be formulated as a constrained nonlinear optimization model having linear and nonlinear constraints. It consists of the coupled set of flow and transport equations describing the physical and chemical phenomena taking place within transient groundwater system, and linear and/or nonlinear objectives of the considered management problem. Other constraints representing local, political, economic and managerial

considerations, and physical boundary conditions are also included in the model. The model may have single or multiple objectives depending upon the requirements of specific cases of regional groundwater management problem. Appropriate restrictions may be placed upon hydraulic heads, water production targets and water quality standards.

The proposed management model is formulated using the embedding technique in order to eliminate the necessity of linking it to an external simulation model. The model consists of a specified objective function, a number of managerial and physical constraints that include actual or imposed boundary conditions, and the finite difference forms of the governing equations. These features of the model are described in the following subsections.

3.5.1 Objective functions

After specifying the system of interest and defining system boundaries, the next step in the formulation of the optimization model is to select a criterion on the basis of which the performance of the system can be evaluated. On the basis of this criterion, the best set of management strategies can be identified within the operating range of interest. The management model may have single or multiple conflicting objectives, hence one or multiple performance measures will be available to define the noninferior solutions. However, in many situations, it may turn out that only one criterion is the primary one and the remaining criteria may be secondary.

These secondary objectives can be achieved through constraints. This chapter describes only single objective based groundwater management problem. The multiple objectives based groundwater management problems are discussed in Chapter 8.

A number of objectives can be defined for regional management of groundwater. These objectives will depend on the case specific situations and requirements. Once the constraints of the model has been specified, it is relatively easy to incorporate various objectives of management as explicit objective functions. In some cases some of the objectives may be included implicitly as constraints.

Two different types of groundwater management problems each having explicitly stated single objective function are considered as the integrated management models. Both management problems are formulated as single objective optimization problem. The first management model deals with a groundwater supply problem, whereas the second management model deals with the containment of contaminant or restoration of the aquifer.

In Model I, the objective is to maximize the sum of temporal and spatial pumping fluxes for the duration of the time horizon of planning. The purpose of this model is to maximize the total amount of pumping from the aquifer for various water supply purposes while meeting the required water quality standards. This objective function can be stated as:

$$\text{Maximize} \quad F_1 = \sum_{k=1}^{nts} \sum_{i,j \in I} (Q_p)_{i,j}^k \tag{3.115}$$

Where, I denotes a set of specified grid locations (i,j). nts is the number of time steps considered within a planning horizon.

In Model II, the objective is to minimize the sum of temporal and spatial pumping fluxes for the duration of the time horizon of planning. The purpose of this model is to minimize the total required amount of pumping in order to control pollutant concentrations at various locations in the aquifer. This objective function is stated as:

$$\text{Minimize} \quad F_2 = \sum_{k=1}^{nts} \sum_{i,j \in I} (Q_p)_{i,j}^k \tag{3.116}$$

3.5.2 Simulation constraints

To simulate the flow and transport processes occurring within the groundwater system, the finite difference forms of the coupled set of flow and transport equations are embedded as equality constraints within the optimization model. These equality constraints enable the management model to provide meaningful, realizable and feasible solution of modeled real world problems. By coupling flow and transport equations and embedding these coupled set of equations into the optimization model, the integrated excitation response of the groundwater system is obtained due to

groundwater stresses and imposed physical and managerial constraints. Incorporation of simulation constraints represented by Equations (3.46) and (3.88) impose all assumptions mentioned in section 3.3.4 on the management model.

3.5.3 Managerial constraints

In addition to simulation constraints, some constraints may be encountered due to local and regional conditions, requirements and operating conditions of the system. Such constraints are referred to as managerial constraints. Some constraints may represent implicit objectives of the system. Many factors determine the quantitative values of the variables associated with these managerial constraints. These factors basically depend upon the various requirements for different kinds of use of water, sustainability and usability of groundwater, and available operating conditions. However, some of these managerial constraints may reflect political necessities and economic impacts, and some may arise due to assumptions associated with the model. These constraints are necessary to be incorporated into the model in order to evolve socially, politically, financially, economically, environmentally and technically feasible management policies. In absence of explicit expressions, these managerial constraints may be expressed in terms of decision variables implicitly. The managerial constraints imposed in this management model are the following:

(i) The temporal and spatial distribution of hydraulic heads are

such that it should not drop below the specified minimum values

$$h_{i,j}^{k} \geq (h_{lb})_{i,j}^{k} \tag{3.117}$$

(ii) The temporal and spatial distribution of hydraulic heads are such that it should not rise above the specified maximum values

$$h_{i,j}^{k} \leq (h_{ub})_{i,j}^{k} \tag{3.118}$$

(iii) Total pumping from a cell at a particular time must satisfy the minimum specified water demand in that cell

$$(Q_p)_{i,j}^{k} \geq (Q_{lb})_{i,j}^{k} \tag{3.119}$$

(iv) Total pumpage from a cell at a particular time should not exceed a specified upper bound

$$(Q_p)_{i,j}^{k} \leq (Q_{ub})_{i,j}^{k} \tag{3.120}$$

(v) The temporal and spatial distribution of concentration of pollutant in the aquifer should not fall below the specified values (usually zero or any other specified value)

$$c^k_{i,j} \geq (c_{lb})^k_{i,j} \tag{3.121}$$

(vi) The temporal and spatial distribution of concentration of pollutant in the aquifer should not exceed the specified threshold values to meet the water quality standards for the intended use

$$c^k_{i,j} \leq (c_{ub})^k_{i,j} \tag{3.122}$$

h_{lb}, Q_{lb}, c_{lb} are the lower bounds on hydraulic head, pumping and concentration, whereas h_{ub}, Q_{ub}, c_{ub} are the upper bounds on hydraulic head, pumping and concentration respectively.

3.5.4 Initial and boundary conditions

Any model of a real world system remains ill defined in the absence of properly specified boundary conditions, and initial conditions (for transient cases). The management models presented here also require specified boundary and initial conditions to obtain physically meaningful solutions. The initial conditions necessary for solution of this model are the distribution of hydraulic head and concentration in the aquifer domain under consideration at the initial time, usually taken as t = 0. Mathematically, it can be expressed as:

$$h(x, y, 0) = f_1(x, y) \qquad \text{in } R \tag{3.123}$$

$$C(x, y, 0) = f_2(x, y) \quad \text{in } R \tag{3.124}$$

Where $f_1(x, y)$ and $f_2(x, y)$ are known functions, and R stands for the aquifer domain under consideration.

The boundary conditions may reflect actual physical boundary conditions existing in the aquifer, or in some cases certain boundary conditions may be imposed on the system as a managerial or political requirement. The physical boundary conditions express the way the considered domain interacts with its surroundings, and these conditions act as physical constraints in the management model. The boundary may be a Dirichlet type (constant head), Neumann type (constant flux) or mixed type called Cauchy type boundary condition. The proposed models are capable of solving three types of boundary conditions: (i) constant head boundary all along the aquifer boundary, (ii) impervious or no flow boundary along the adjoining sides of constant head boundary, and (iii) mixed boundary consisting of patches of constant head and impervious boundary zones all along the aquifer boundary. Mathematically, it can be expressed as:

Boundary condition type 1:

$$h(x, y, t) = f_3(x, y) \quad \text{on } B_i; \quad i = 1, 2, 3, 4 \tag{3.125}$$

$$C(x, y, t) = f_4(x, y) \quad \text{on } B_i; \quad i = 1, 2, 3, 4 \tag{3.126}$$

Boundary condition type 2:

$$h(x, y, t) = f_3(x, y) \qquad \text{on } B_i; \quad i = 1, 2 \tag{3.127}$$

$$C(x, y, t) = f_4(x, y) \qquad \text{on } B_i; \quad i = 1, 2 \tag{3.128}$$

$$\frac{\partial}{\partial n}\Big(h(x, y, t)\Big) = 0 \qquad \text{on } B_i; \quad i = 3, 4 \tag{3.129}$$

$$C(x, y, t) = 0 \qquad \text{on } B_i; \quad i = 3, 4 \tag{3.130}$$

Boundary condition type 3:

$$h(x, y, t) = f_5(S_1) \qquad \text{on } B_i; \quad i = 1, 2, 3, 4 \tag{3.131}$$

$$C(x, y, t) = f_6(S_2) \qquad \text{on } B_i; \quad i = 1, 2, 3, 4 \tag{3.132}$$

$$\frac{\partial}{\partial n}\Big(h(x, y, t)\Big)\Bigg|_{S_3} = 0 \qquad \text{on } B_i; \quad i = 1, 2, 3, 4 \tag{3.133}$$

$$C(S_4, t) = 0 \qquad \text{on } B_i; \quad i = 1, 2, 3, 4 \tag{3.134}$$

Where $f_3(x, y)$, $f_4(x, y)$, $f_5(S_1)$ and $f_6(S_2)$ are known functions. B stands for boundary, index, i stands for the side of the rectangular finite difference network approximating the aquifer domain under consideration, and n refers to the normal direction of the boundary. S_1, S_2, S_3 and S_4 are the specified set of coordinates (x, y) corresponding to the finite difference network. The functions f_3,

These constraints can be expressed as:

$$(Q_p)^k_{i,j} = 0; \quad \text{if } (\delta_p)_{i,j} = 0; \qquad (i,j) \in S_5 \tag{3.135}$$

$$(\delta_r)_{i,j} = 0; \qquad (i,j) \in S_6 \tag{3.136}$$

$$(Q_p)^k_{i,j} \geq 0; \quad \text{if } (\delta_p)_{i,j} = 1; \qquad (i,j) \notin S_5 \tag{3.137}$$

$$(\delta_r)_{i,j} = 1; \qquad (i,j) \notin S_6 \tag{3.138}$$

S_6

Where S_5 and S_5 denote sets of cell locations in which pumping is not desired and recharge is zero throughout the planning horizon respectively.

3.5.6 Lower and upper bounds

The lower bounds on hydraulic heads are chosen such that the aquifer does not become unconfined. The upper bounds on hydraulic heads are chosen such that the area does not become waterlogged. These bounds may be modified also as per desired political or managerial requirements if appropriate.

The lower bound on pumping can be estimated based on the water required for irrigation from groundwater resource. It depends upon the water requirement for a crop in a particular agroclimatic region and the irrigation practice to be adopted if groundwater is needed for the irrigation. Thus, the lower bound on pumping can be computed

from the expression:

$$Q_{1b} = \frac{(C_u - R_e + W_1)\ A_c\ \eta_g\ PF_i}{86400\ B\ \eta_a\ \eta_c} \qquad (3.139)$$

Where C_u, R_e, W_1, B and A_c represent respectively consumptive use of water by crop (m), effective rainfall (m) in the area during crop period, water required for leaching (m), base period (days) of crop and area (m^2) under crop. η_a η_c and η_g are respectively water application efficiency, water conveyance efficiency and proportion coefficient for groundwater use. η_g accounts for the conjunctive irrigation practice to be adopted. It is the ratio of water required for irrigation from groundwater resource and total water requirement for the crop during the entire base period of the crop. In a modified management model explicitly formulated for optimal conjunctive use of groundwater and surface water, η_g should represent a decision variable. PF_i denotes peak factor for irrigation water demand to account the surplus requirement of water during germination or kor period.

The consumptive use of water for a crop is estimated by Hargreaves class A pan evaporation method which uses Christiansen formula for the determination of class A pan evaporation. The details are available in Michael (1978). The lower bound computed from the above expression reflect the average pumping rate required

during the base period of the crop. Thus, either a time varying or a time average value of lower bound on the pumping from different cells can be estimated from the above expression depending upon the cropping pattern existing or proposed in the area during the planning horizon.

If the pumping is desired for the municipal, domestic and/or industrial purposes, the lower bound on pumping is computed from the following expression:

$$Q_{lb} = \frac{Q_d \; PD \; A_d \; PF_d \; \eta'_g}{8.64 \times 10^{11} \; \eta_d} \tag{3.140}$$

Where Q_d, PD, A_d and PF_d represent the average water supply demand (lpcd), population density (persons/hectare), area for which demand is needed (m^2), and peak factor to account for surplus demand during peak period respectively. η'_g and η_d denote proportion coefficient for groundwater use and water distribution efficiency respectively. η'_g accounts for the conjunctive practice to be adopted to satisfy water supply need. It is the ratio of the volume of groundwater used for domestic purposes to the total volume of water requirement for domestic use. In a modified management model explicitly formulated for optimal conjunctive use of groundwater and surface water, η'_g should represent a decision variable. η_d accounts for the friction losses in distribution pipes network. In case of other than domestic use, i.e. the industrial, commercial or municipal use, the lower bound is computed on the basis of its population equivalent.

If the pumping is required for more than one purpose, the lower bound will be the sum of the requirements for all purposes. It should be noted here that in case of some other specific groundwater management problems, i.e. salinity removal or management under water deficit, formulated in a different way, the same quantities may be stated as upper bounds instead. If the objective is only to control the pollution during the planning period such that the spatial distribution of pollutants satisfy the desired quality standard for a crop, domestic, industrial or municipal use, the lower bound on pumping becomes simply nonnegative.

The upper bounds on pumping are generally based on the pumping capacity of the pump to be installed. It can be estimated from the following expression:

$$Q_{ub} = \frac{75\ P\ \eta_p\ n_p}{\gamma\ h_{max}} \tag{3.141}$$

Where P, h_{max} and γ represent respectively pump capacity in h.p., maximum head of water to be lifted in m. and specific weight of water in kg/m^3. η_p and n_p denote efficiency of pump and number of pumps installed in the area to lift the water.

The upper bounds on concentrations depend upon the specific use. These bounds are imposed as per the water quality standard needed for the particular use. This standard may be different in different areas and at different time. The lower bounds on

concentrations will be generally specified as nonnegative only.

3.5.7 System parameters and system information

The estimated values of aquifer parameters are also required for solution of the model. These spatial parameters are hydraulic conductivity, saturated thickness which may vary also with time, storage coefficient, thickness of the leaky layer and hydraulic head in the source bed. The effective porosity, longitudinal and transverse dispersivities, and other geological information if any are also required to solve the model.

If the aquifer is leaky, information about the quality of leakage entering into the aquifer is necessary. The concentration of pollutant in leakage may vary with space and time. The locations of waste disposal or injection wells if any are also required in order to model the system more adequately and to assess the impact of these natural or man-made influences. The temporal and spatial information about the quality of recharge through injection wells in addition to recharge rate are required to solve the model. All these information which constitute required estimates of parameter values and other input conditions describe the model completely and depict the history of all the processes occurring within the system and their influences on the system.

3.5.8 Assumptions

In addition to the assumptions mentioned in section 3.3.4, some more assumptions are associated with the proposed model. These assumptions arise due to the processes followed for the discretization of the governing equations and formulation of the management model. Assumptions enumerated below must be carefully evaluated in conjunction with the assumptions mentioned in section 3.3.4 before applying the model to a field problem:

1. The first order decay constant is same in both liquid and solid phase.
2. Retardation factor is assumed equal to one.
3. The molecular diffusion is assumed negligible in comparison to convective diffusion.
4. The point pumping from a cell represent the sum of point pumping from the various wells located within a cell.
5. The point recharge to a cell represent the sum of point recharge to the various wells located within a cell.

Assumptions 4 and 5 effectively allow more than one pumping or recharge wells in a cell, or a combination of both pumping and recharge wells in a cell. The latter seems to be more realistic in case of larger grid size because recharge does not merely reflect industrial disposal but, rural, urban, domestic, or municipal waste also. In case of more than one recharge wells in a aquifer, the concentration of pollutant in recharge to a cell is estimated based on conservation of mass principle.

3.6 Nonlinearities in the Model

Nonlinearities in the model arise due to presence of products of unknown concentration and unknown velocity field in advective and dispersive transport terms. The velocity field is unknown because pumping rates are decision variables and therefore, pumping rates are unknown. Nonlinearities may also arise due to the nature of objective functions considered. Commonly groundwater solute transport is accompanied by chemical reactions in the moving water as well as complex interactions of solutes with the porous media. These reaction may be homogeneous or heterogeneous. Nonlinearities are encountered due to multicomponent chemical interactions in the moving water and with the porous media (Rubin and James 1973, Valocchi et al. 1981, Jennins et al. 1982). However, the proposed models do not incorporate any nonlinear chemical interactions. The methodology presented here is however, equally applicable to those models incorporating these nonlinearities due to chemical interactions. The proposed models can be applied in such cases by modifying simulation equations. The computational complexities will no doubt increase if such processes are also incorporated.

3.7 Proposed Method of Solution

Once the simulation constraints are embedded in the management model, it results in a constrained nonlinear optimization model. The resulting optimization model is a highly complex multivariable nonlinear programming problem. To find the optimal solution, the

constrained problem can be transformed into a sequence of unconstrained problems using either the Interior Penalty Function Method (IPFM) or the Exterior Penalty Function Method (EPFM). The proposed methodology utilizes EPFM to convert the constrained optimization problem into a sequence of unconstrained optimization problems. The transformed objective function is called composite objective function or pseudo objective function. After transforming the constrained optimization problem into a sequence of unconstrained optimization problems, the solution is obtained by solving these unconstrained problems. Discussions on the methods available to solve the multivariable nonlinear unconstrained problem and selection of the appropriate one to implement in the present methodology are presented in the next chapter.

3.7.1 Exterior penalty function method

The exterior penalty function method converts the constrained optimization problem into unconstrained one. For the conversion of constrained to unconstrained one, the objective function is expanded by including the penalty function which is a function of constraints and a penalty parameter. The resulting objective function, composite objective function is expressed as:

$$\phi(x, r) = f(x) + \Omega(r, g(x), h(x)) \tag{3.142}$$

Where r is a set of penalty parameters and $\Omega(.)$, the penalty

function is a function of r and the constraint functions. x denotes the set of decision variables, g(.) and h(.) represent the equality and inequality constraints respectively. $\phi(.)$ and f(.) represent respectively the composite objective function and the original objective function. The penalty function may be quadratic, logarithmic, inverse, or bracketed one. It depends upon the constraints involved.

The main advantage of EPFM is that it is not necessary to provide an initial feasible solution to start the optimization process. In this method, the sequence of unconstrained optima may lie in the infeasible region but finally it converges to an optimal feasible solution. This method thus eliminates the difficulties of finding the initial feasible point. This particular approach is very much suitable for the solution of this management problem, because, finding a initial feasible solution is extremely difficult. The penalty function method is also very suitable when embedding technique is used, because it can handle a large number of equality constraints which result from embedding the simulation constraints directly into the optimization model. However, the efficiency of this method depends on the efficiency of the unconstrained minimization method used.

3.7.2 Composite objective functions and constraints

The composite objective functions which constitute the unconstrained minimization problems for the proposed management

models can be expressed as:

$$\phi_1(h, Q_p, C, r) = - F_1 + \frac{1}{r} \sum_{n=1}^{2} g_n(h, Q_p, C) \tag{3.143}$$

$$\phi_2(h, Q_p, C, r) = F_2 + \frac{1}{r} \sum_{n=1}^{2} g_n(h, Q_p, C) \tag{3.144}$$

Where

$$g_1(h, Q_p, C) = \sum_{k=1}^{nts} \sum_{i,j \in I} \left[(g_f)_{i,j}^k \right]^2 \tag{3.145}$$

$$g_2(h, Q_p, C) = \sum_{k=1}^{nts} \sum_{i,j \in I} \left[(g_t)_{i,j}^k \right]^2 \tag{3.146}$$

The functions $(g_f)_{i,j}^k$ and $(g_t)_{i,j}^k$ represent the equality constraints defined by left hand side terms of Equations (3.46) and (3.88) respectively. The bounds on the decision variables remain the same as described by inequalities (3.117) to (3.122). The boundary conditions and other physical constraints also remain the same as expressed by Equations (3.123) to (3.138)

3.7.3 Estimation of the penalty parameter

The composite objective functions (Equations 3.143 and 3.144) obtained for the proposed management models are minimized for different values of penalty parameter to get the optimal solution.

To start the sequence of unconstrained search, it is necessary to choose an initial value for the penalty parameter, and to devise a strategy for updating this value after each unconstrained search. This is necessary to force convergence of the sequence of optimal solutions towards the global optimal value. If a proper value of penalty parameter is not selected, the unconstrained problems may become difficult to solve, and computational termination may occur as a result of failure of the unconstrained optimization method. The selection of penalty parameter depends upon the size and type of the optimization problem, and on the order of the numerical values of the objective function and the constraints involved in the optimization. The initial value of the penalty parameter and a strategy to update it can be established by conducting a large number of exploratory tests.

3.7.4 Significance of dimensionless numbers

There are three dimensionless numbers which are encountered in the modeling of groundwater management models. These numbers are Reynolds number, Peclet number and Courant number. Reynold number for the flow through porous media is defined as:

$$R_e = \frac{q\ d}{\nu} \tag{3.147}$$

Where d is some representative microscopic length characterizing the solid matrix and ν is the kinematic viscosity of the fluid. In terms

of velocity, Reynold number can be expressed as:

$$R_e = \frac{v\ n_{eff}\ d}{\nu} \tag{3.148}$$

The average velocity, v, through the pores of the porous media is determined from the Darcy's law. Reynold number is computed to see whether Darcy's law is valid or not. Because the management model is also based on the Darcy's law, its validity must be satisfied in terms of the Reynolds number. For the Darcy's law to be valid, Reynolds number should be less than or equal to one, although Reynolds number upto 10 may be acceptable. However, R_e more than one is rarely encountered in flow through aquifers. During the search for optimum solution, it is noticed that Darcy's law remains valid and the obtained optimum solution represents a valid flow system. In two-dimensional flow, v is given by:

$$v = \sqrt{v_x^2 + v_y^2} \tag{3.149}$$

This number in cartesian coordinates can be expressed as:

$$R_{e_x} = \frac{v_x\ n_{eff}\ d}{\nu} \tag{3.150}$$

$$R_{e_y} = \frac{v_y\ n_{eff}\ d}{\nu} \tag{3.151}$$

Peclet number, P_e is defined as:

$$P_e = \frac{L\ v}{D_d}$$

$$\approx \frac{d\ v}{D_d} \tag{3.152}$$

Peclet number in cartesian coordinates can be expressed as:

$$P_{e_x} = \frac{d\ v_x}{D_d} \tag{3.153}$$

$$P_{e_y} = \frac{d\ v_y}{D_d} \tag{3.154}$$

Where L is some characteristic length of the pores and D_d is the coefficient of molecular diffusion of the solute in the liquid phase. In a dilute system, D_d is approximately equal to 10^{-9} m^2/s. It is Peclet number by which molecular diffusion is coupled with mechanical dispersion as discussed in section 3.3.3. On the basis of Peclet number, dominance of molecular diffusion and mechanical dispersion can be assessed. If Peclet number is less than 0.4, molecular diffusion predominates, as the average flow velocity is vary small ($\alpha_L v << D_d T^*$). The effects of mechanical dispersion and molecular diffusion are of the same order of magnitude if Peclet number lies between 0.4 and 5. If Peclet number is greater than 5,

mechanical dispersion predominates. These results are based on the experimental results obtained by Pfannkuch (1963) and Saffman (1960) for one dimensional flow through unconsolidated porous media (Bear and Verruijt, 1987). Computation of this number gives an assessment of the results in context of incorporated assumptions in the model.

Courant number, C_r is defined as:

$$C_r = \frac{v \, \Delta t}{\Delta s} \tag{3.155}$$

In two-dimensional flow, Δs is given by:

$$\Delta s = \sqrt{\Delta x^2 + \Delta y^2} \tag{3.156}$$

Courant number in cartesian coordinates can be expressed as:

$$C_{r_x} = \frac{v_x \, \Delta t}{\Delta x} \tag{3.157}$$

$$C_{r_y} = \frac{v_y \, \Delta t}{\Delta y} \tag{3.158}$$

This number plays a vital role in the selection of grid sizes Δx and Δy, and time step Δt to avoid computational error. The Courant number should be always less than one during the search and this condition should be also satisfied at the optimum point. Mathematically this condition is expressed as:

$$C_r \leq 1 \tag{3.159}$$

However, this condition is not strictly required to be satisfied at every iteration during the search processes of optimization, but it should be guaranteed that the obtained optimum solution satisfies this inequality and deviation is not much during the search processes. This is a modeling requirement, otherwise pollutant may cross the cell before it is considered for the analysis ($v\,\Delta t > \Delta s$). Because, the embedding approach used in this model is based on implicit scheme, the significance of Courant number in determining the stability of solutions is not relevant. However, Peclet and Courant number conditions have to be met to control oscillations and numerical error (Ferreira, 1988; Sudicky, 1989; Lee and Kitanidis, 1991).

3.8 SUMMARY

This chapter described the modeling of regional groundwater management problems. Two groundwater management models describing (i) supply problem and (ii) contaminant containment problem or aquifer restoration problem were formulated as integrated management models which consider both quality and quantity aspects together by coupling the flow and transport equations. The methods of solution for the groundwater management problems have been analyzed and a suitable and efficient method, i.e., the exterior penalty function method has been described. This chapter dealt with the complete

modeling of the groundwater management problems starting from the formulation to development and solution of the models. The next chapter describes the algorithms for solution of the resulting large sized unconstrained nonlinear optimization problems and necessary modifications made in these algorithms to solve the proposed integrated management models.

APPLICATION OF NONLINEAR PROGRAMMING USING PATTERN SEARCH METHODS

CHAPTER 4

APPLICATION OF NONLINEAR PROGRAMMING USING PATTERN SEARCH METHODS

Once a multivariable constrained nonlinear optimization problem is transformed into a multivariable unconstrained nonlinear optimization problem, the optimum can be obtained by using any of the methods available to solve an unconstrained minimization problem. The methods available for unconstrained minimization problems are equally applicable for unconstrained maximization problems. Generally the algorithms for minimization are also used for maximization problems after multiplying the objective function by a negative sign. The special characteristic of transformed unconstrained minimization problem is that the solution vector need not satisfy any constraint. But the order of violation of constraints should be negligible.

The methods that have been devised for the solution of the

unconstrained minimization problem can be classified broadly into two categories: (i) direct search (nongradient) methods, and (ii) descent (gradient) methods. The direct search methods require only objective function evaluations, whereas descent methods require the evaluations of first, second and/or higher order derivatives of the objective function in addition to function evaluations. All the methods have some advantages and disadvantages over others. It is sure that no one method or class of methods can solve all problems with equal efficiency and accuracy. Applicability of methods to solve a given problem depends on certain special requirements and factors such as: dimensionality, CPU time, accuracy, differentiability, inconsistency, analytical expressions for derivatives or difference approximations for derivatives, experimentation for step sizes to eliminate roundoff and truncation errors etc. Therefore, it requires some analyses of the methods available and the method to be adopted for the solution depending on the characteristics of the problem at hand. All unconstrained minimization methods are iterative in nature and hence they start from an initial trial solution and proceed towards the optimum point in a sequential manner. The detailed descriptions and discussions of various methods are available in Fox (1971), Murray (1972), Reklaitis et. al. (1983), Arora (1989) and Rao (1992).

Direct methods are based on the assumption that the objective function to be minimized is continuous, and gradient of objective function may or may not exist but certainly is not available. Howev-

er, these methods can be used to solve the problems where gradient of objective function does exist. These methods are also used when gradient of objective function is a complex vector function of the decision variables. It should be mentioned here that the objective function is assumed unimodal in the domain of interest. Therefore, application of these methods to multimodal functions may lead to local optimum point.

Direct methods are classified broadly into heuristic techniques and theoretically based techniques. The heuristic techniques are search methods constructed from geometric intuition for which no performance guarantees other than empirical results can be stated. The theoretically based techniques, on the other hand, do have a mathematical foundation that allows performance guarantees, such as convergence, to be established at least under restricted conditions.

Two direct methods, the Hooke-Jeeves method (Hooke and Jeeves, 1966) and Powell's conjugate direction method (Powell, 1964) are analyzed here in details as these two methods are implemented for the solution of the proposed integrated management models. Both the methods are pattern search methods. The Hooke-Jeeves method is based on heuristic technique, whereas Powell's conjugate direction method employs a theoretically based technique. The common characteristic of these two methods is that computationally they are relatively uncomplicated, hence easy to implement.

After transforming the multivariable constrained nonlinear optimization models for groundwater management problems into a sequence

of multivariable unconstrained nonlinear optimization models, the solutions are obtained by solving these unconstrained models. The various methods (Davidon 1959, Fletcher and Powell 1963, Fletcher and Reeves 1964, Powell 1964, Hooke and Jeeves 1966, Polak and Ribiere 1969, Broyden 1970, Fletcher 1970, Shanno 1970) available for solving the unconstrained problems are Hooke-Jeeves (HJ), Powell's Conjugate Direction (PCD), Fletcher-Reeves (FR), Polak-Ribiere (PR), Davidon-Fletcher-Powell (DFP) and Bryoden-Fletcher-Shanno (BFS). Details are available in Reklaitis et al. (1983), Arora (1989) and Rao (1992). All of these methods except HJ and PCD require derivatives of the composite objective function. It is difficult to obtain the explicit analytical expressions for the derivatives of the composite objective function which is highly nonlinear, complex and a large multivariable function in the groundwater management models discussed in Chapter 3. To find the derivatives numerically will require more computer time and approximations. The descriptions of HJ and PCD methods, the rationale for their selection, and necessary modifications made in the algorithms to make them suitable for the solution of the proposed management model are discussed in the following sections.

4.1 HOOKE-JEEVES METHOD

The pattern search method of Hooke and Jeeves utilizes a sectioning technique. It employs exhaustive searches by the use of exploratory and pattern moves based on heuristic rules. It is

observed on the basis of computation that the HJ method can be successfully employed to obtain an optimal solutions of the proposed groundwater management models. The choice of using the HJ method in conjunction with EPFM is motivated by the fact that the HJ method eliminates many computational difficulties associated with solving the large nonlinear optimization problem.

Implementation of HJ method is simple and straight forward. It is not adversely affected by sparse constraint matrices. Computational difficulties like inconsistencies between composite objective function and derivative values, nondifferentiability, and invalid arguments do not arise in this method. These difficulties may arise in other methods of unconstrained nonlinear optimization, especially in gradient based methods. The other advantage of the HJ method is that it requires less computer memory as it is not required to store information regarding search directions during the exploratory search or pattern move.

4.1.1 Description of the Hooke-Jeeves algorithm

It consists of two kinds of moves: exploratory move and pattern move. The exploratory move is performed to examine the local behaviour of the function and to locate the direction of any sloping valleys that might be present. The pattern move utilizes the information generated in the exploratory move to step rapidly along the valley. It is an accelerating move along the valley and regulated by some heuristic rules.

specified step size in each coordinate direction of decision space taking one variable at a time. If the function value decreases, the step is considered successful. Otherwise, the step is retraced and replaced by a step in the opposite direction, which in turn is retained depending upon whether it succeeds or fails. When all N coordinates have been investigated, the exploratory move is completed and the resulting point is termed a base point. The pattern move consists of a single step from the present base point along the line from the previous to the current base point. The general procedure with particular reference to a minimization problem can be described by the following steps:

Steps:

1. Define:

   Initial solution vector to start the search process, x^o

   Perturbation vector (initial step sizes), Δx^o

   Step reduction factor, $\alpha > 1$

   Acceleration factor, $\beta \geq 1$

   Termination parameter, $\varepsilon > 0$

2. Compute the objective function at x^o, $\psi(x^o)$;

   and set initial basic value of objective function, $\psi^b = \psi(x^o)$,

   and initial basic decision variable vector, $x^b = x^o$

3. Perform exploratory search to obtain the new temporary base point as:

Let the optimal value of objective function, $\psi^{*} = \psi^{b}$;

and optimal solution vector, $x^{*} = x^{b}$

$$\psi^{*} = \psi_i^{+} \text{ and } x_i^{*} = x_i^{+}; \quad \text{if } \psi_i^{+} = \psi(x_i^{+}) < \psi^{b}; \text{ where } x_i^{+} = x_i + \Delta x_i \tag{4.1}$$

$$\psi^{*} = \psi_i^{-} \text{ and } x_i^{*} = x_i^{-}; \quad \text{if } \psi_i^{-} = \psi(x_i^{-}) < \psi^{b}; \text{ where } x_i^{-} = x_i - \Delta x_i \tag{4.2}$$

$$\psi^{*} = \psi_i \text{ and } x_i^{*} = x_i; \quad \text{if } \psi_i < \min.\ (\psi_i^{+}, \psi_i^{-}) \tag{4.3}$$

Where i refers to index for the decision variables, i.e. vector components. This process is continued for all the decision variables, i.e. i = 1, 2, 3, . . ., n; where n denotes number of decision variables. The final updated solution vector indicates a point in decision space which indicates a direction of objective function improvement.

4. Was exploratory search successful ?

Yes: Go to 6

No : Continue

5. Check for termination:

Is $|\Delta x| < \varepsilon$?

$$\Delta x_i = \frac{\Delta x_i}{\alpha}; \qquad i = 1, 2, 3, . . ., n \tag{4.4}$$

go to 3

6. Perform pattern move:

$$x_p^{k'+1} = x^{k'} + \beta \, (x^{k'} - x^{k'-1}) \tag{4.5}$$

Where $x^{k'-1}$ and $x^{k'}$ are previous and current base points respectively. $x_p^{k'+1}$ refers to pattern move point. In fact, superscript represents the stage of decision vector, and hence, $x^{k'}$ represents the best point after exploratory search at k'^{th} stage, and $x^{k'-1}$ serves as a base point for the pattern move at k'^{th} stage.

7. Perform exploratory search using $x_p^{k'+1}$ as the base point (as mentioned in Step 3); Let the best solution vector be $x^{k'+1}$. Basically, it represents a new or next base point.

8. Is $\psi(x^{k'+1}) < \psi(x^{k'})$?

Yes: set $x^{k'-1} = x^{k'}$;

$$x^{k'} = x^{k'+1}; \tag{4.6}$$

go to 6 (4.7)

No : Go to 5

In the above procedure, the objective function represents the composite objective function for the proposed groundwater management models. The decision variable vector comprises of all pumping, hydraulic head and concentration variables.

4.1.2 Actual implementation for the management problem

To implement HJ algorithm described in section 4.1.1 for the solution of the groundwater management models, the following modifications must be made in the algorithm:

Modification 1

In step 4, the total number of decision variables are needed to decide whether exploratory search was successful or not. It is understood failure only when, no improvement in objective function value is achieved after performing exploratory search for all decision variables at a stage. Any improvement in objective function value due to change in any of the decision variables is termed as a successful exploratory search. Thus, total number of decision variables must be computed accurately. Otherwise, search process may proceed in a wrong direction. In some specific cases, pumping may be desirable from only some specified locations of study area rather than from all the cells of finite difference network. In such cases, total number of decision variables (tnodv) is computed as:

$$\text{tnodv} = \left[2\ (nc-2)(nr-2) + \sum_{i,j \in S_7} (\delta_p)_{i,j} \right] \text{nts} \tag{4.8}$$

Where nc and nr, nts, and S_7 denote respectively number of columns and number of rows in a finite difference network, number of time steps, and a set of locations in a finite difference network from which pumping is desired.

Modification 2

Groundwater management models like the proposed management model generally have three classes of decision variables. These are pumping (or withdrawal), hydraulic head and concentration of a pollutant. The number of variables in each class depends upon the discretization network, pumping locations and number of time frames considered in the planning horizon. The magnitudes of decision variables in a class are almost of the same order, but decision variables in different classes will differ in order of magnitude. Thus different class of decision variables have different representative step sizes, reduction factors, acceleration factors and termination parameters. However, for the decision variables belonging to one class, these optimization parameters need not be different. This is essential to overcome the possibility of scaling problem.

Thus, new optimization parameters defined for different classes of variables are α_q, α_h, α_c (reduction factors); β_q, β_h, β_c

(acceleration factors) and ε_q, ε_h, ε_c (termination parameters); where q, h and c represent the class of decision variables for pumping, hydraulic head and concentration respectively. The step sizes for pumping, hydraulic head and concentration variables thus become Δq, Δh and Δc respectively. Therefore exploratory search is performed using step length Δq for pumping variables, Δh for hydraulic head variables and Δc for concentration variables. This modification will expedite the search. The formulae for pattern move in step 6 of section 4.1.1 take the following forms:

<u>For pumping variables</u>

$$(\underline{P})_p^{k'+1} = (\underline{P})_p^{k'} + \beta_q \left[(\underline{P})^{k'} - (\underline{P})^{k'-1}\right] \tag{4.9}$$

<u>For hydraulic head variables</u>

$$\underline{h}_p^{k'+1} = \underline{h}^{k'} + \beta_h \left[\underline{h}^{k'} - \underline{h}^{k'-1}\right] \tag{4.10}$$

<u>and For concentration variables</u>

$$\underline{C}_p^{k'+1} = \underline{C}^{k} + \beta_c \left[\underline{C}^{k'} - \underline{C}^{k'-1}\right] \tag{4.11}$$

Where $\underline{P}$, $\underline{h}$ and $\underline{C}$ denote the class vectors for pumping, hydraulic head and concentration variables respectively. The superscript represents the stage of the decision variable during the search

process.

In step 5 of section 4.1.1, the reduction of step length is made as follows:

<u>For pumping variables</u>

$$\Delta q = \frac{\Delta q}{\alpha_q} \tag{4.12}$$

<u>For hydraulic head variables</u>

$$\Delta h = \frac{\Delta h}{\alpha_h} \tag{4.13}$$

<u>and For concentration variables</u>

$$\Delta c = \frac{\Delta c}{\alpha_c} \tag{4.14}$$

Execution is terminated whenever the following inequalities are simultaneously satisfied:

$$\Delta q \leq \varepsilon_q \tag{4.15}$$

$$\Delta h \leq \varepsilon_h \tag{4.16}$$

$$\Delta c \leq \varepsilon_c \tag{4.17}$$

odification 3

All groundwater management models possess lower and upper ounds on decision variables. These bounds are either explicitly tated or implicitly incorporated during the formulation of the model. The algorithm presented in section 4.1.1 does not incorporate these bounds. If bounds were treated separately as inequality constraints during the transformation of the constrained problem into unconstrained one, this issue would have become redundant. But an efficient way of handling these bounds is simply to restrict the range of search of interest. In doing so, the pattern move should be checked for violation of bounds and corrective modifications should be made in the moves if it occurs. It is necessary to prevent the infeasible solution, even though the search starts from an initial feasible solution. This situation in which a pattern move becomes infeasible is shown in Fig. 4.1.

Fig. 4.1a shows how the decision variable, x_1 crosses the upper bound prescribed for x_1 during the pattern move. The crossing of decision variable, x_1 beyond the lower bound prescribed for x_1 after pattern move is shown in Fig. 4.1b. $(x_1)_p$, $(x_1)_{ub}$ and $(x_1)_{lb}$ represent respectively variable x_1 after pattern move, upper bound on decision variable x_1 and lower bound on decision variable x_1. The decision vector x_1 denotes here any decision variable of any class, pumping, hydraulic head or concentration. If this crossing is permitted, the finally obtained optimum solution may no longer be a feasible solution. If this situation is not corrected, solution may

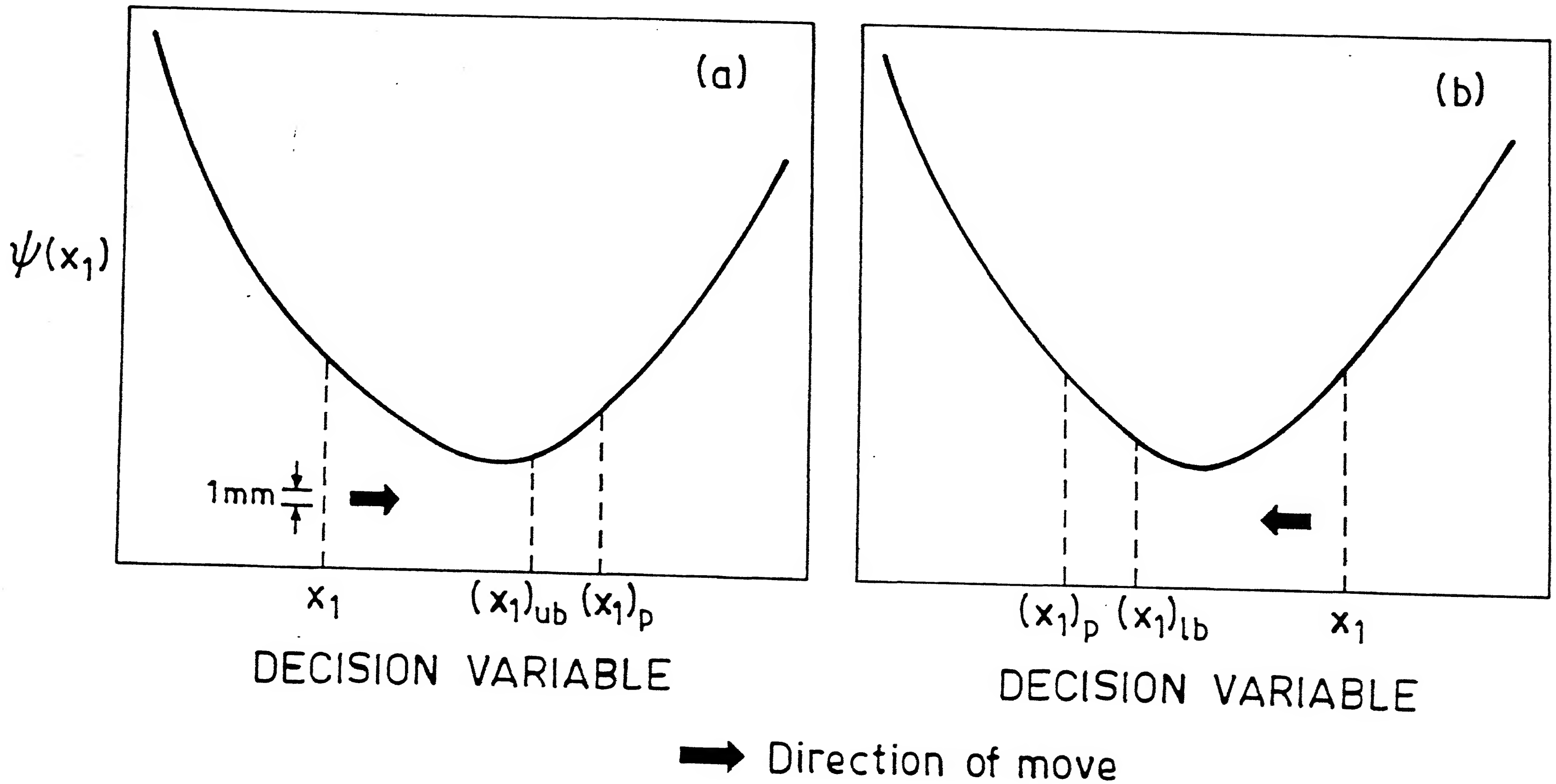


Fig. 4.1 Representation of infeasible pattern moves : (a) upper bound (b) lower bound .

converge to an infeasible region or may yield nonpositive values of decision variables. To eliminate this problem, the acceleration factor for that particular decision variable is made zero and thus pattern move becomes ineffective for this particular decision variable. Mathematically it can be expressed as:

$$\beta_q = 0; \qquad \text{if } \left[(Q_p)^k_{i,j}\right]^{k'}_p > (Q_{ub})^k_{i,j} \tag{4.18}$$

$$\beta_h = 0; \qquad \text{if } \left[(h)^k_{i,j}\right]^{k'}_p > (h_{ub})^k_{i,j} \tag{4.19}$$

$$\beta_c = 0; \qquad \text{if } \left[(C)^k_{i,j}\right]^{k'}_p > (C_{ub})^k_{i,j} \tag{4.20}$$

Modification 4

It is observed during the development of the software that sometimes pattern move fails. It implies that the value of objective function on the basis of decision variables obtained after pattern move is higher than that has been obtained from the last exploratory search. In such a situation, the value of objective function obtained from exploratory search instead of pattern move is made the basis for comparison in the next exploratory search to find the direction of improvement. If exploratory search fails, the pattern move is deemed a failure. At this juncture, the algorithm returns to the last successful exploratory search and the process begins again

with new reduced step sizes. Mathematically it can be described as:

Let $x^{k'}$ be decision variable vector after exploratory search. A pattern move is made at $x^{k'}$, resulting vector, $x_p^{k'+1}$. ψ $(x^{k'})$ will serve as a basis for the exploratory search if the following inequality holds true:

$$\psi\ (x_p^{k'+1}) > \psi\ (x^{k'}) \tag{4.21}$$

If exploratory search fails, pattern move is deemed a failure. At this point, the algorithm returns to decision vector $x^{k'}$ and search process is continued with reduced step sizes, again starting from the exploratory search anew.

4.2 POWELL'S CONJUGATE DIRECTION METHOD

Powell's Conjugate Direction (PCD) method is a pattern search method and is based on the objective function evaluations only. This algorithm effectively uses the history of the iterations to build up directions for acceleration and at the same time avoids degenerating to a sequence of coordinate searches. It is based upon the model of a quadratic objective function and thus has a theoretical basis. Powell's method has been found to be the most efficient direct search method because of the quadratic convergence property. This property is expected to speed up the convergence process even for nonquadratic functions. Choosing a quadratic model for the algorithm is due to the following two reasons:

(i) It is the simplest type of nonlinear function to minimize, and hence any general technique must work well on a quadratic function if it is to have any success with a general nonlinear function.

(ii) Near the optimum, all nonlinear functions can be approximated by as quadratic function because in the Taylor's series expansion, the linear part must vanish. Hence, the behaviour of the algorithm on the quadratic function will give some indication of how the algorithm will converge for general nonlinear functions.

It is felt that the PCD method can be successfully employed to obtain an optimal solution to the proposed management problem. The choice of using the PCD method in conjunction with EPFM is motivated by the fact that the PCD method eliminates many computational difficulties associated with solving the large nonlinear optimization problem. The use of PCD method is simple and straight forward. It is not adversely affected by sparse constraint matrices, inconsistencies between composite objective function and derivative values, nondifferentiability and invalid arguments that may arise in other methods of unconstrained nonlinear optimization.

However, one drawback of this method is that it requires more computer memory in comparison to the HJ method, as the search directions are stored during each cycle. The direction vector requires a large space for storing the vector components in order to handle large sized nonlinear optimization problem. Secondly, the

search directions may become dependent or almost dependent in the course of numerical computation. It occurs whenever the optimum step length in any particular direction happens to be zero. The detailed comparison of HJ and PCD methods on the basis of the solutions of the management problems is discussed in Chapter 7.

4.2.1 Description of the Powell's conjugate direction algorithm

It consists of cyclic use of one dimensional searches and generation of search direction vectors. In one dimensional search, Quadratic Fitting (QFIT) is employed to find the optimal step length. QFIT again assumes a quadratic function at optimum point. It is basically a Successive Quadratic Estimation Method (SQEM) at which optimum point is obtained using a quadratic model and this point is modified till it matches with the general nonlinear function under consideration near the optimal point (Fig. 4.2). For one dimensional search, other methods like Cubic Fitting (CFIT), Newton-Raphson, Bisection, Secant methods are also available; but all these methods require evaluation of derivatives. To avoid the use of a gradient based technique, these methods are not employed here for one dimensional search.

9 Bracketing the optimum in the QFIT technique can be done by any of the methods available: Equal Interval Search Technique (EIST), Interval Halving Search Technique (IHST), Golden Section Search Technique (GSST) and Fibonacci Search Technique (FST). The general procedure of the PCD algorithm utilizing QFIT in conjunction with

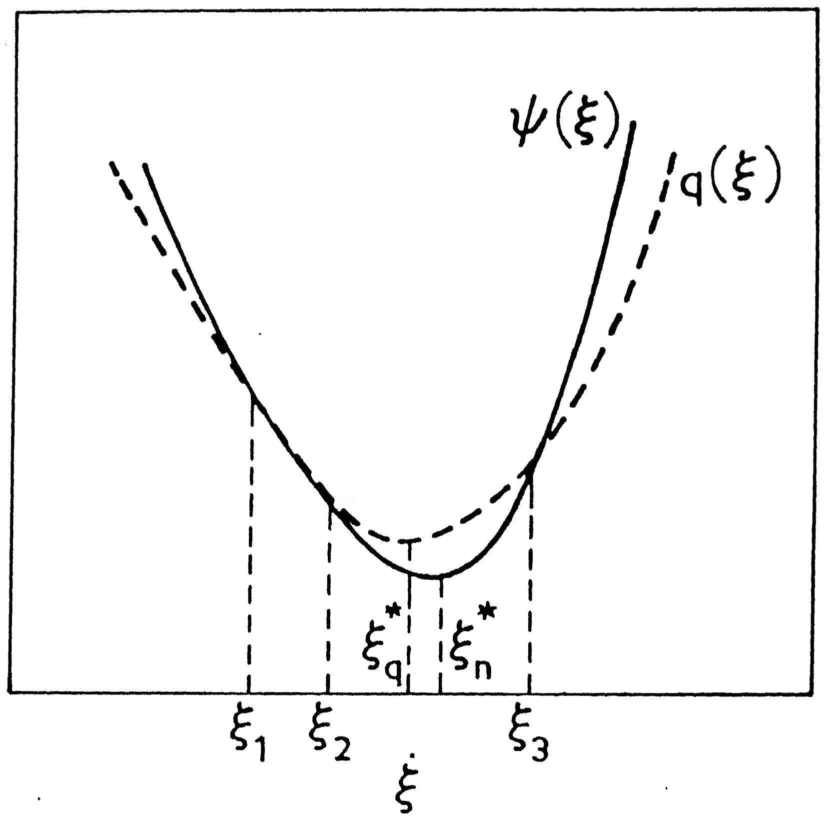


Fig. 4.2 Quadratic approximation of nonlinear function at optimum.

equal interval search technique is outlined below. For quadratic fitting, the following functional form is used:

$$q(x) = a_o + a_1 x + a_2 x^2 \tag{4.22}$$

Where x denotes any decision variable and q (x) is an approximated quadratic function of the actual nonlinear function ψ (x) for the decision variable x. a_o, a_1 and a_2 are the coefficients to be determined for each one dimensional nonlinear function.

Steps:

1. Define :

   initial solution vector (starting point), x^o

   set of n linearly independent directions, e^i; i = 1, 2, . . n

   convergence parameter for the decision variables in one dimensional optimal search, ε_{1dv}

   convergence parameter for the function in one dimensional optimal search, ε_{1df}

   termination parameter to stop execution, ntermi

   initial solution for the decision variable in one dimensional optimal search, ξ

   step size for the decision variable in one dimensional optimal search, $d\xi$

2. Minimize along the n+1 directions as one dimensional search by letting e^n as the first and last search. Optimum step length in

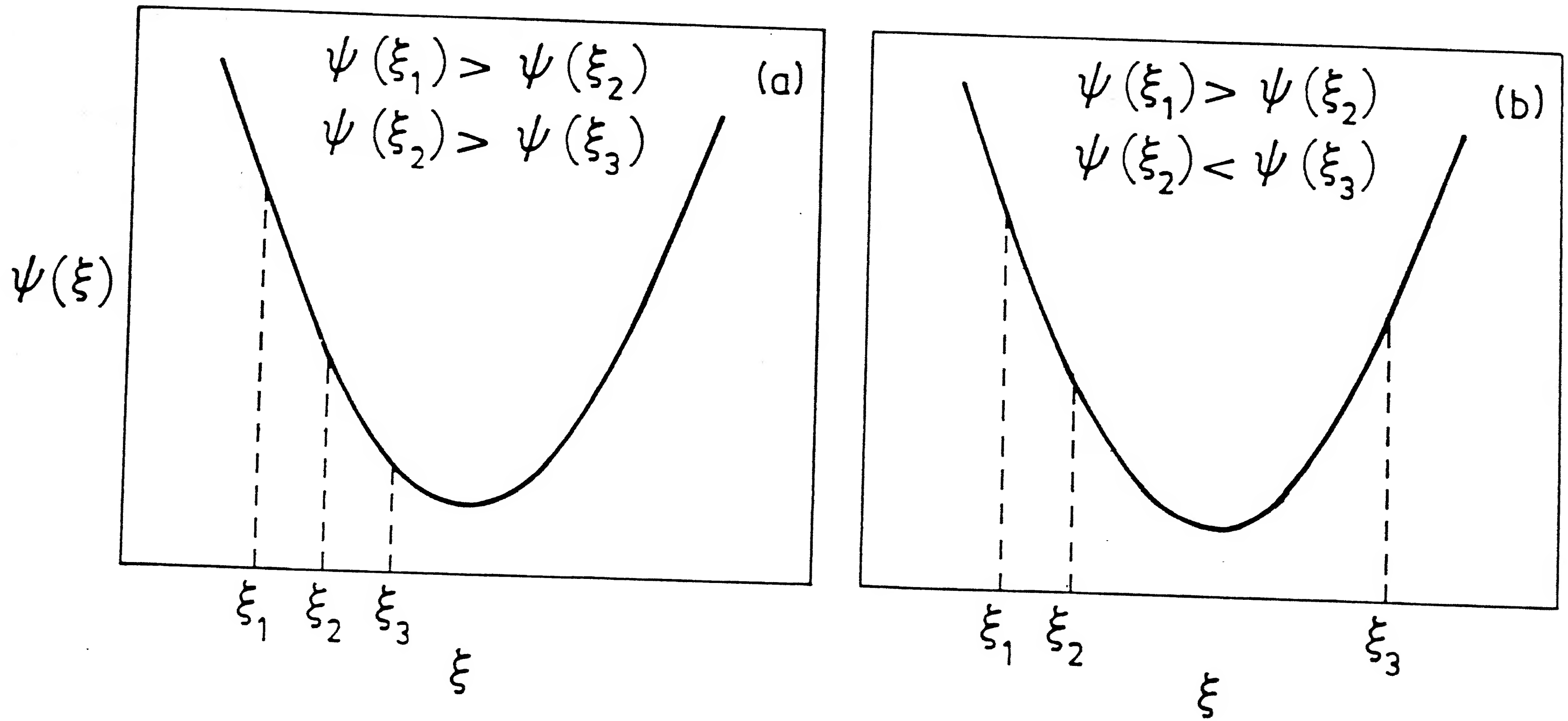


Fig. 4.3 Schematic representation of bracketing the optimum : (a) possibility 1; (b) possibility 2.

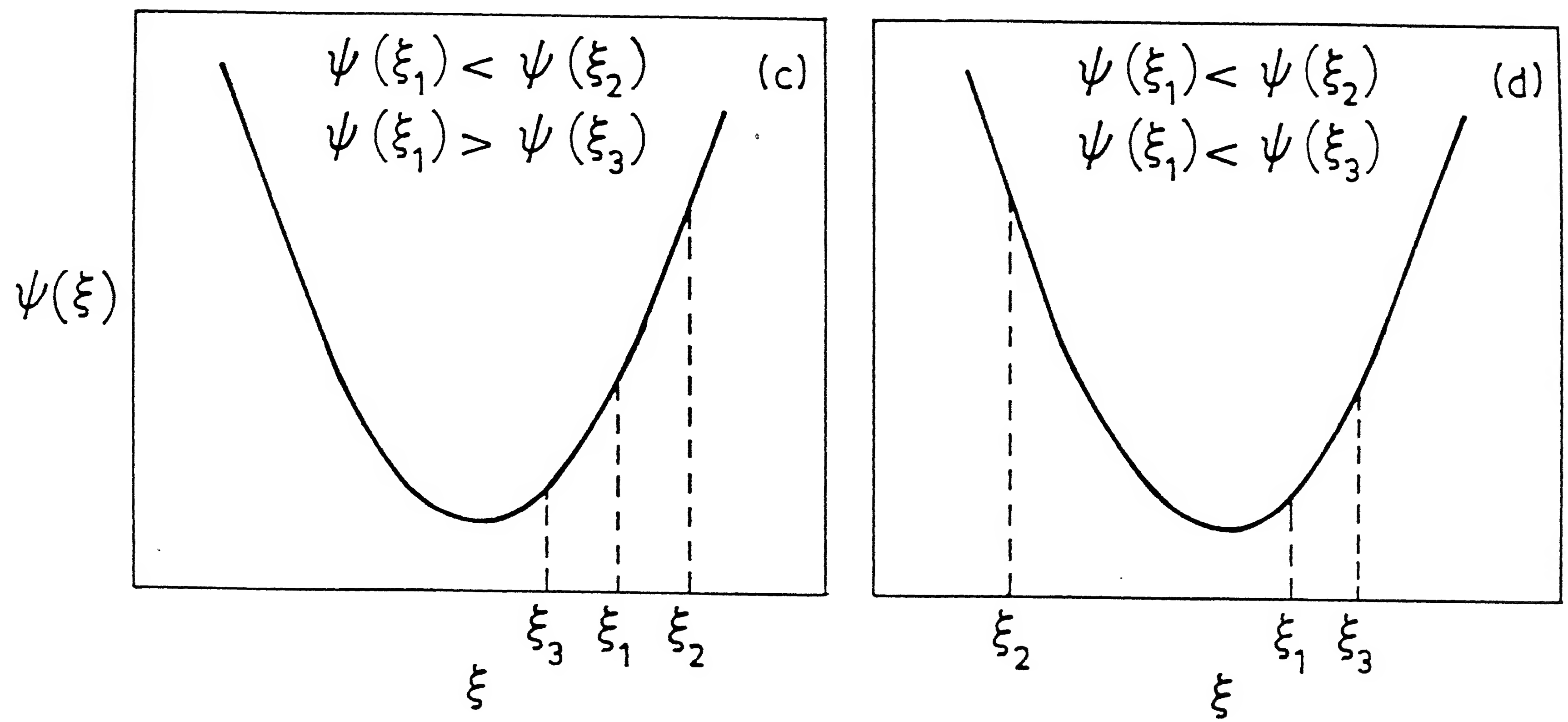


Fig. 4.3 Schematic representation of bracketing the optimum (c) possibility 3; (d) possibility 4.

2a $\xi_3 = \xi_1 + 2\, d\xi$ (4.30)

Is $\psi(\xi_2) > \psi(\xi_3)$?

Yes : set

$$\xi_1 = \xi_2 \tag{4.31}$$

$$\xi_2 = \xi_3 \tag{4.32}$$

$$\psi(\xi_1) = \psi(\xi_2) \tag{4.33}$$

$$\psi(\xi_2) = \psi(\xi_3) \tag{4.34}$$

go to 2a

No : continue

One dimensional optimization, QFIT

2c Finding the optimum step length, ξ^* and optimum functional value, $\psi(\xi^*)$

$$\xi_m = \xi_2 \tag{4.35}$$

$$\psi(\xi_m) = \psi(\xi_2) \tag{4.36}$$

$$a_2 = \frac{1}{\xi_3 - \xi_2}\left[\frac{\psi(\xi_3) - \psi(\xi_1)}{\xi_3 - \xi_1} - \frac{\psi(\xi_2) - \psi(\xi_1)}{\xi_2 - \xi_1}\right] \tag{4.37}$$

$$a_1 = \frac{\psi(\xi_2) - \psi(\xi_1)}{\xi_2 - \xi_1} - a_2(\xi_1 + \xi_2) \tag{4.38}$$

$$a_o = \psi(\xi_1) - a_1\, \xi_1 - a_2\, \xi_1^2 \tag{4.39}$$

$$\xi^* = -\frac{a_1}{2\, a_2} \tag{4.40}$$

The four possibilities arise in order to eliminate the region of noninterest. These are shown in Fig. 4.4.

Is $\xi_2 < \xi^*$?

Yes : go to 2d

No : go to 2e

2d Is $\psi(\xi_2) < \psi(\xi^*)$?

Yes : $\xi_3 = \xi^*$ (4.41)

$\psi(\xi_3) = \psi(\xi^*)$ (4.42)

go to 2f

No : $\xi_1 = \xi_2$ (4.43)

$\xi_2 = \xi^*$ (4.44)

$\psi(\xi_1) = \psi(\xi_2)$ (4.45)

$\psi(\xi_2) = \psi(\xi^*)$ (4.46)

go to 2f

2e Is $\psi(\xi_2) < \psi(\xi^*)$?

Yes : $\xi_1 = \xi^*$ (4.47)

$\psi(\xi_1) = \psi(\xi^*)$ (4.48)

go to 2f

No : $\xi_3 = \xi_2$ (4.49)

$\xi_2 = \xi^*$ (4.50)

$\psi(\xi_3) = \psi(\xi_2)$ (4.51)

$\psi(\xi_2) = \psi(\xi^*)$ (4.52)

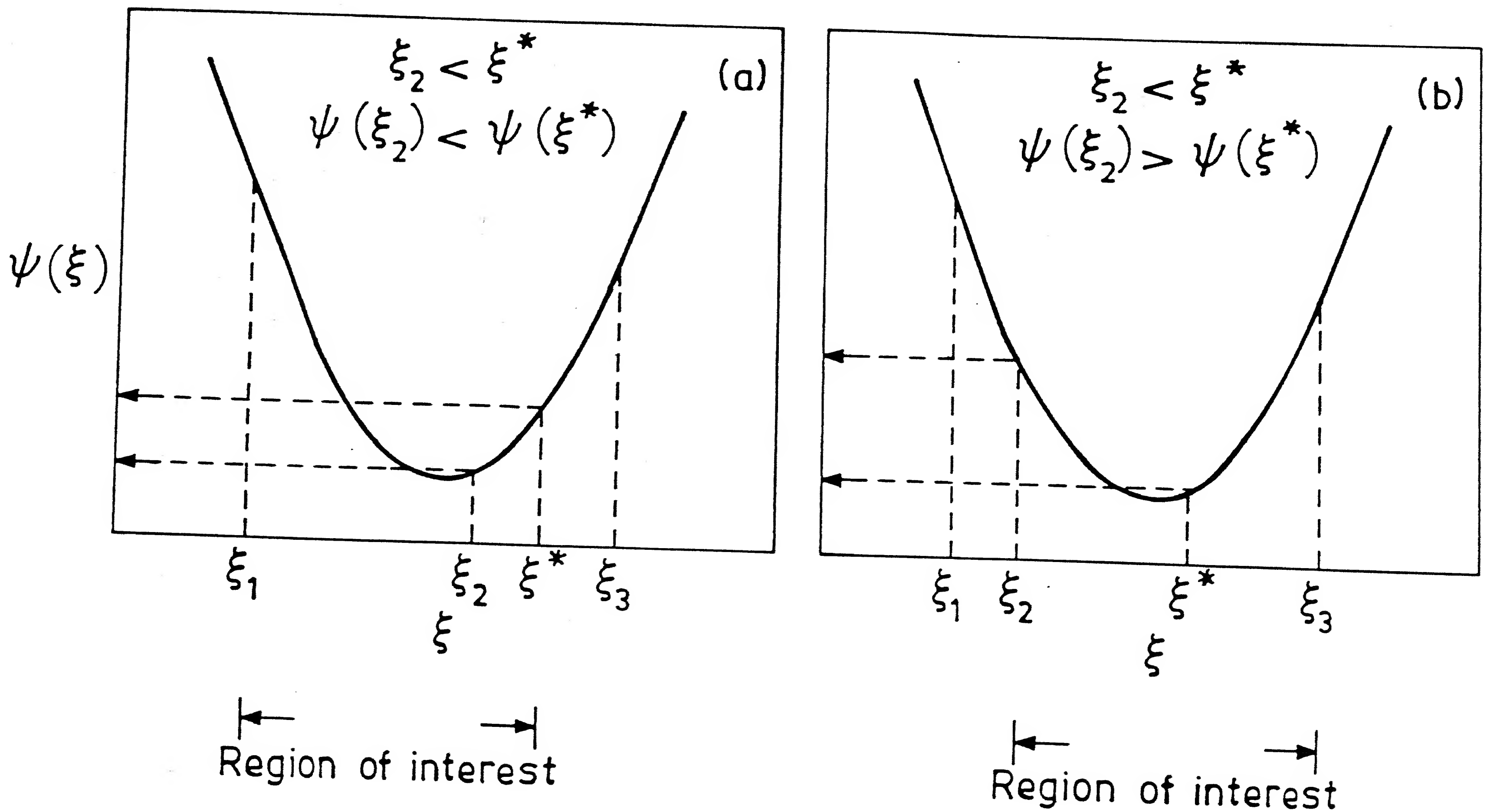


Fig. 4.4 Identification of region of interest (a) possibility 1; (b) possibility 2.

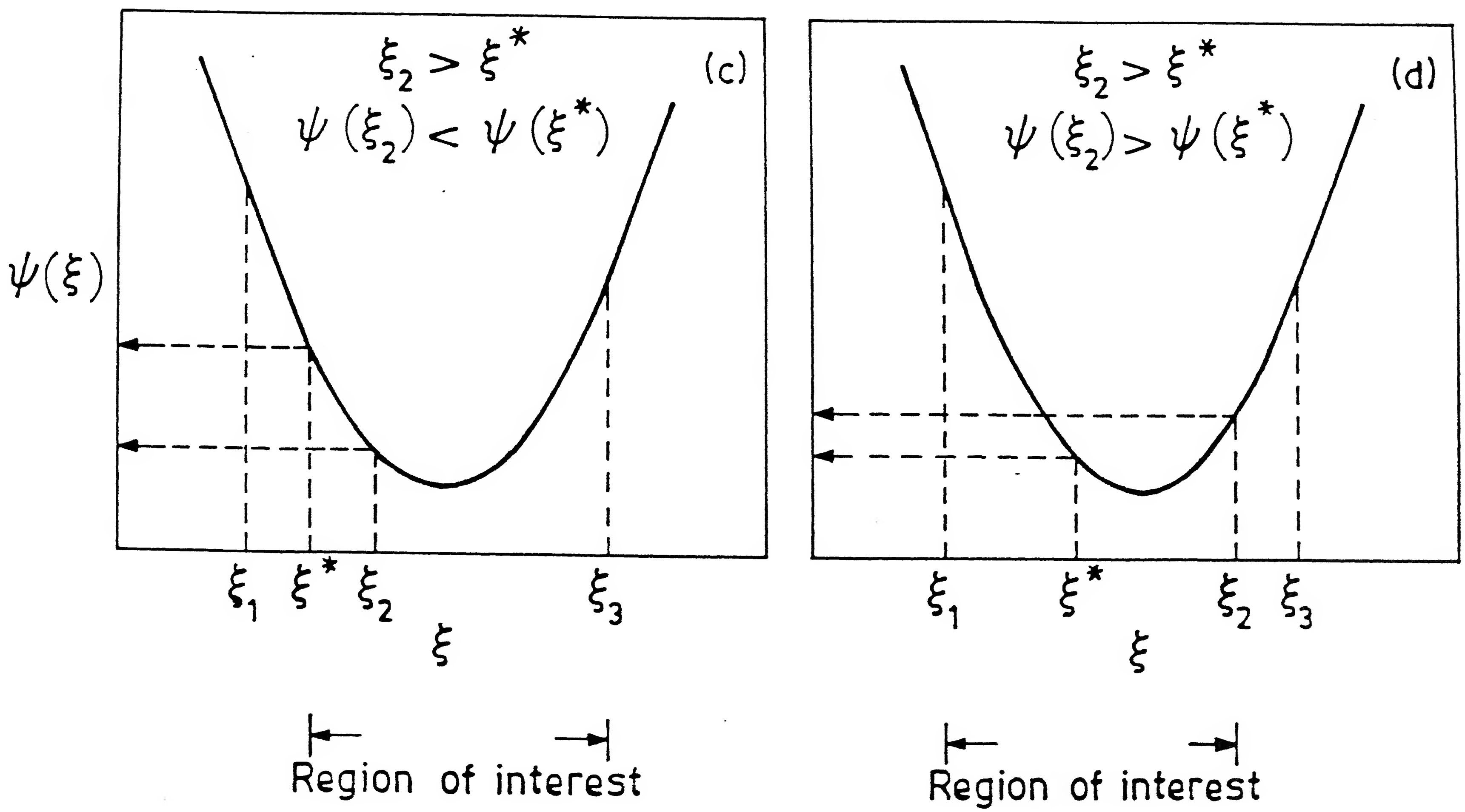


Fig. 4.4 Identification of region of interest (c) possibility 3; (d) possibility 4.

go to 2f

2f check the termination

(a) Is $$\left| \frac{\psi(\xi_m) - \psi(\xi_2)}{\psi(\xi_2)} \right| \leq \varepsilon_{1df} \ ? \qquad (4.53)$$

(b) Is $$\left| \frac{\xi_m - \xi_2}{\xi_2} \right| \leq \varepsilon_{1dv} \ ? \qquad (4.54)$$

If both (a) and (b) are satisfied,

go to 2g

Otherwise,

update ξ_m and $\psi(\xi_m)$

go to step 2c

2g store x and ψ (x) corresponding to ξ_2, an optimal solution in one dimensional search.

This entire process is repeated for all n+1 direction vectors

3. Form the new conjugate directions:

$$e^{n+1} = x^{n+1} - x^{1} \qquad (4.55)$$

$$e_{mag} = \left| e^{n+1} \right| \qquad (4.56)$$

$$e^{n+1} = e^{n+1} / e_{mag} \qquad (4.57)$$

Superscript represents the stage. Stage refers to the completion of that particular one dimensional search in the cycle.

4. Replace the direction vector e^1 by e^{n+1} and reset all the direction vectors to form a new set of conjugate directions. go to step 2

5. The process is repeated till the convergence is achieved. The termination criterion based on convergence is specified by the following inequality:

$$\text{nstage} \geq \text{ntermi} \tag{4.58}$$

Where 'nstage' denotes the number of stages performed to obtain the optimal value of objective function.

The direction vector, e^i is basically a row matrix of the direction vector matrix, e having n x n dimensions, where n is the number of decision variables. In the above procedure, $\psi(\xi)$ refers to the evaluation of objective function (composite objective function for proposed groundwater management models) at $x + \xi e^i$.

4.2.2 Actual implementation for the management problem

In order to implement the PCD algorithm stated in section 4.2.1 to solve the groundwater management models for its solution, the following modifications in the algorithm are necessary:

Modification 1

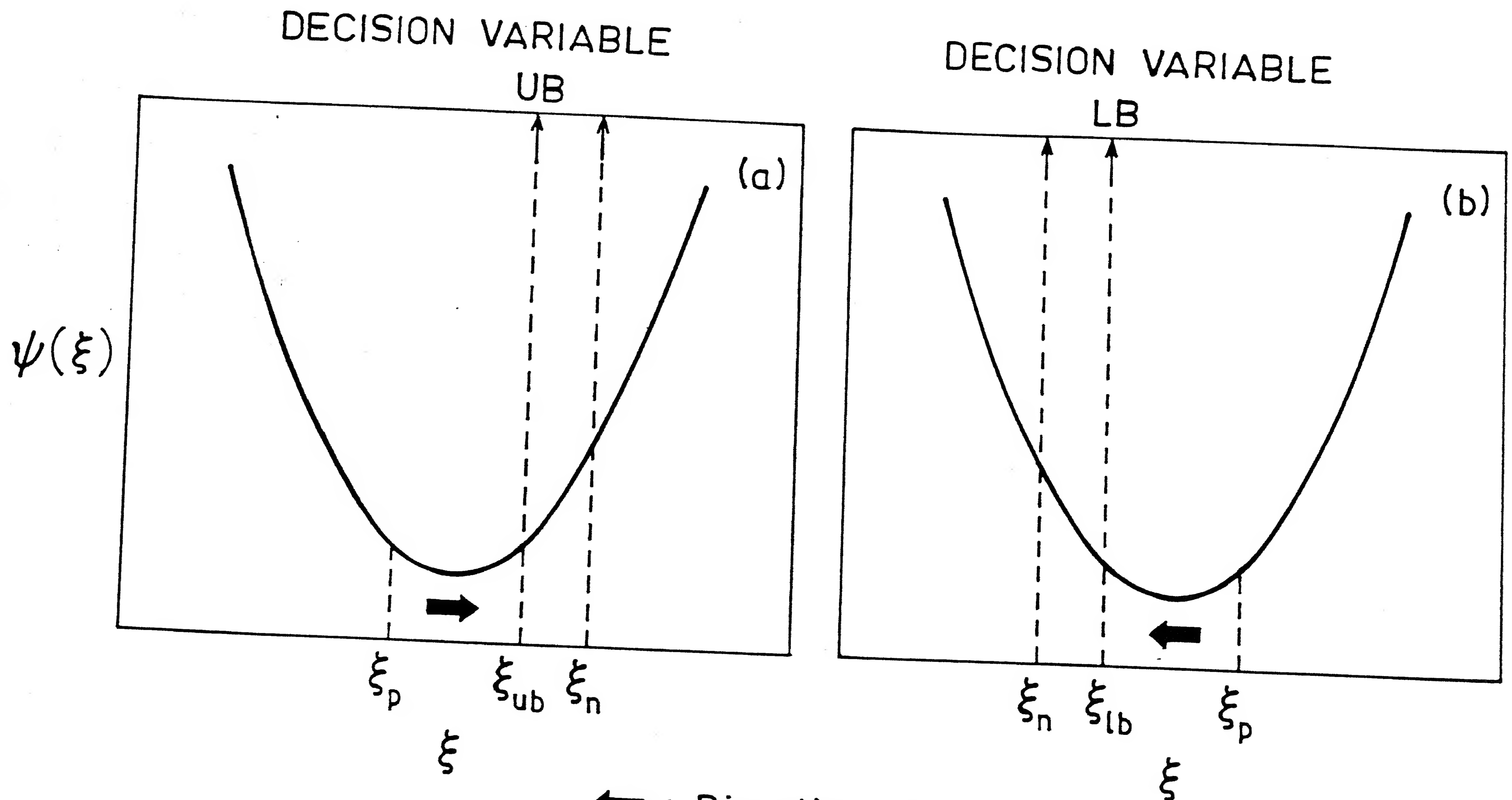
To perform one dimensional search, ξ_1, ξ_2 and ξ_3 are obtained using ξ and $d\xi$ to bracket the optimum point as discussed in the section 4.2.1. Groundwater management models including the proposed ones generally have three classes of decision variables: (i) pumping, (ii) hydraulic head, and (iii) pollutant concentration. The order of magnitude of decision variables belonging to a class are almost of the same order, but order of magnitudes of decision variables belonging to different classes differ appreciably.

Therefore, values of ξ and $d\xi$ should be different for these three classes of variables in order to accelerate the finding of bracketing points and to avoid the computational problems which may arise due to the presence of bounds on decision variables. This is also necessary to overcome the scaling problem. Thus, the new seed values for bracketing the optimum point are ξ_h, ξ_q, ξ_c, $d\xi_h$, $d\xi_q$ and $d\xi_c$. h, q and c denote the class of decision variables for pumping, hydraulic head and concentration respectively. The step 2 is modified accordingly.

Modification 2

All groundwater management models possess lower and upper bounds on decision variables. These bounds are either explicitly stated or implicitly incorporated during the formulation of the model. The algorithm of PCD method presented in section 4.2.1 does not incorporate the bounds. If bounds were treated separately as inequality constraints during the transformation of the constrained problem into unconstrained one, this issue would become redundant. But an efficient way of handling these bounds are simply to restrict the region of search. This reduces the computation time and also eliminates the possibility of computational difficulties which may arise if these inequalities were treated separately during the conversion from constrained to unconstrained problem. To keep the search within the region of interest, a check is introduced whenever values of decision variables are adjusted according to ξ during the one dimensional search and estimation of ξ^*. It restricts the direction move towards infeasible region and thus, ensures the decision variables to be within the feasible region. Otherwise, the infeasible directional move may lead to a solution which will not be optimum or feasible. Such situations are shown in Fig. 4.5.

Fig. 4.5a and 4.5b show how the computed step length during bracketing, or finding the optimum step length, crosses the upper or lower bounds specified for the decision variables respectively. ξ_{ub} and ξ_{lb} represent the value of ξ corresponding to upper and lower bounds on decision variables respectively. ξ_p and ξ_n denote the



: Direction of move
UB : Upper bound on decision variable
LB : Lower bound on decision variable

Fig. 4.5 Representation of infeasible directional moves for (a) upper bound (b) lower bound.

preceding and next values of ξ respectively. UB and LB stand respectively for upper and lower bounds on decision variable corresponding to ξ_{ub} and ξ_{lb}. These situations may be encountered in any of the four classes of bracketing explained in Fig. 4.3 or, while finding the optimum step length explained in Fig. 4.4. To eliminate the infeasibility problem, the next value of ξ (ξ_n) is made equal to the previous one (ξ_p), i.e.

$$\xi_n = \xi_p \tag{4.59}$$

In the bracketing process or during the iteration process for getting the optimum step length, this modification may yield following three conditions:

$$(1)\ \xi_1 = \xi_2 \tag{4.60}$$

$$(2)\ \xi_2 = \xi_3 \tag{4.61}$$

$$(3)\ \xi_1 = \xi_3 \tag{4.62}$$

Whenever this condition is obtained, the optimum step length is computed from the following expression to avoid the possibility of getting infinite or indeterminate values which may occur in the computation of either a_1, a_2 or ξ^*:

$$\psi\ (\xi^*) = \min.\ [\ \psi\ (\xi_1),\ \psi\ (\xi_2),\ \psi\ (\xi_3)\ ] \tag{4.63}$$

$$\xi^* = \xi \text{ corresponding to } \psi(\xi^*) \tag{4.64}$$

Modification 2 is applied in the light of Modification 1.

Modification 3

After incorporation of the modifications 1 and 2 in the PCD algorithm, solutions of the proposed management models can be obtained. During the finding of the solutions of the models, it is observed that solutions sometimes converge and sometimes diverge. Even though some divergence in the solution occurs, it converges after some more cycles. But this cyclic behaviour of convergence and divergence may lead to a solution that converges to an inferior one (ψ_{io}) compared to a superior solution (ψ_{so}) obtained in an earlier cycle. This situation is shown graphically in Fig. 4.6.

To eliminate this problem, the direction vectors are tracked at each cycle. The whole procedure of optimization is resumed and the solution is sought with the initial direction vector from the last identified superior point, whenever any divergence is observed after the completion of a cycle. Mathematically it can be stated as:

$$\text{if } \psi(\xi)\Big|_{[e] = [e]_{ng}} > \psi(\xi)\Big|_{[e] = [e]_{pg}} \tag{4.65}$$

$$[e]_{ng} = [e]_{initial} \tag{4.66}$$

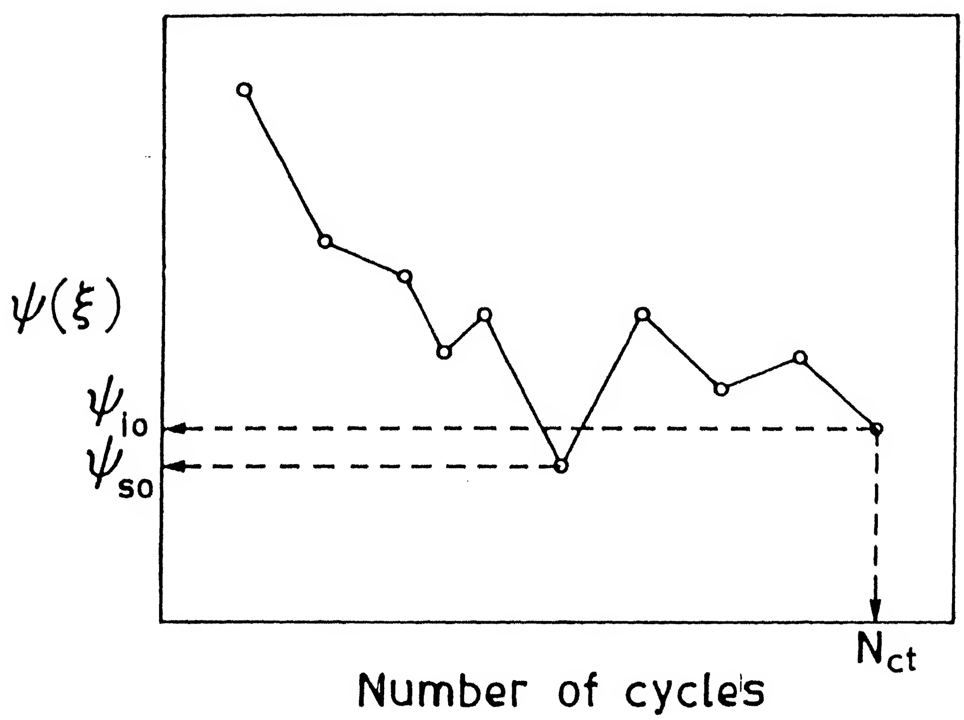


Fig. 4.6. Convergence to an inferior solution due to cyclic behaviour of convergence and divergence.

Where suffix ng and pg refer to newly generated and previously generated respectively.

Modification 4

The value of ntermi to be assigned in the input to terminate the execution is estimated from the following equation, otherwise the computational procedure will hang:

$$\text{ntermi} = (\text{number of decision variables} + 1) \times \text{any integer value} + 1 \tag{4.67}$$

Any integer number here represents the number of cycles desired to be performed in order to obtain the optimum solution. Total number of decision variables is computed using the Equation (4.8).

The quadratic functions require only n^2 line searches to obtain an optimum solution. The number of line searches necessary to obtain the optimum will be generally more than n^2 for nonquadratic functions. It may happen in quadratic functions also. It is because, the one dimensional search may approximate the optimum step length instead of finding the exact optimum due to some numerical computation problems. Thus, the subsequent directions will not be conjugate. Therefore, the method will require more number of iterations for achieving the overall convergence. In case of nonquadratic nonlinear functions, this approximation add to the complexity. However, the method will converge to a local optimum at

a superlinear rate (Reklaitis et al., 1983; Rao, 1992).

The modifications mentioned above are incorporated in the development of the computer code for the solution of the groundwater management models. In addition, for both HJ and PCD algorithms, the boundary conditions as well as other physical constraints discussed in Chapter 3 are incorporated. The problems encountered during the course of the development of the software for the solution of the proposed management models and their remedial measures are discussed in Chapter 7.

4.3 SUMMARY

This chapter focused on the nonlinear programming techniques to solve multivariable unconstrained nonlinear optimization problems. Discussions also focused on the selection of a particular method for the solution of the groundwater management models. The algorithms of Hooke-Jeeves method and Powell's conjugate direction method with quadratic fitting are described in detail. The necessary modifications which must be incorporated to solve the groundwater management problems are described and critically examined. This chapter together with Chapter 3 provides detailed description of the mathematical modeling of regional integrated groundwater management problems including solution techniques to obtain optimum strategies. The groundwater management models formulated in Chapter 3 are solved using the exterior penalty function method in conjunction with Hooke-Jeeves and Powell's algorithms. The performance of the coded

algorithms using EPFM in conjunction with HJ algorithm, and EPFM in conjunction with PCD algorithm to solve the large sized multivariable constrained nonlinear groundwater management models is discussed in the next chapter.

PERFORMANCE EVALUATION OF THE IMPLEMENTED ALGORITHMS

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CHAPTER 5
PERFORMANCE EVALUATION OF THE IMPLEMENTED ALGORITHMS

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After presenting the conspectus and motivation of the present study in the first and second chapters, the third and fourth chapters were devoted to the description of the formulation, development and solution of the groundwater management models. This chapter deals with the performance evaluation of the implemented algorithms for its accuracy and validity. The performance of the algorithms are also evaluated for solving the groundwater management models.

A computer code written in FORTRAN has been developed for exclusively solving the groundwater quality and quantity management problems involving nonlinear objective functions and nonlinear constraints. The developed computer program, NLOGM (Nonlinear Optimizer for Groundwater Management) is capable of solving transient integrated management problems involving either

conservative, radioactive or any other degradable pollutant obeying linear rate of decay. It is coded in two versions. In the first version, solution of multivariable constrained nonlinear groundwater management problems is based on the exterior penalty function method in conjunction with Hooke-Jeeves algorithm. The second version of the program employs the solution technique based on the exterior penalty function method in conjunction with Powell's conjugate direction method. This approach utilizes quadratic fitting for one dimensional search and equal interval search technique for bracketing the optimum in one dimensional search. The program can be used for three types of boundary conditions: (i) constant head boundary, (ii) impervious or no flow boundary, and (iii) mixed boundary consisting of patches of constant and impervious boundary zones. The two-dimensional advective-dispersive-diffusive-degradable transport equation is considered for the migration of pollution plumes in a two-dimensional flow through a heterogeneous anisotropic leaky confined aquifer system. The salient features of the developed computer code, NLOGM is enumerated in Appendix I.

To test the computational correctness of the coded algorithms, some mathematical problems with known exact solutions are solved using the developed computer codes and then compared with the exact solutions. In addition to this, effect of discretization used in the modeling, and sensitivity of objective function to penalty parameter and initial solution are also presented and discussed in this chapter. These analyses are essential to evaluate the performance of

the implemented algorithms for solving the multivariable constrained nonlinear integrated management models.

5.1 TESTING OF THE DEVELOPED OPTIMIZATION ALGORITHMS

The validity of the solutions of multivariable constrained nonlinear optimization algorithms depends upon the correctness of the solutions obtained using coded algorithms for a given problem. In addition, the validity of the solution of a given management system depends on the accuracy of modeling the system in terms of mathematical equations and also the estimated parameter values and boundary conditions. In fact, the validity of the solution obtained for the constrained optimization problem depends on the accuracy and efficiency of implemented unconstrained techniques. It is so because, constrained nonlinear problems are solved as a sequence of unconstrained nonlinear problems as discussed in Chapter 3 in details. Therefore, some constrained and some unconstrained nonlinear mathematical optimization problems are solved and compared with exact solutions to validate the developed codes.

5.1.1 Testing of implemented HJ algorithm

In order to test the computational correctness of the first version of the coded algorithm (EPFM & HJ), a simple test problem is utilized. This test problem can be stated as:

$$\text{Minimize} \quad F_1' = -3803.84 - 138.08\, x_1 - 232.92\, x_2 + 123.08\, x_1^2$$

$$+ 203.64\, x_2^2 + 182.25\, x_1 x_2 \qquad (5.1)$$

The values of α, β and ε for both decision variables, x_1 and x_2 are assumed 2, 1 and 0.0001 respectively. The minimization process is started with 1.0 and 0.5 as initial guesses for x_1 and x_2. The necessary minor modifications are made in the coded algorithm to solve this test problem.

The optimal values of the objective function, decision variables and final step sizes after 10 reduction of step sizes are given in Table 5.1. The results obtained by Kuester and Mize (1973) using HJ method are also tabulated for comparison. This comparison (Table 5.1) appears satisfactory in establishing the correctness of the optimization code developed. A few other test problems are also evaluated, but not reported here. These evaluations also establish the correctness of the computer code.

5.1.2 Testing of implemented PCD algorithm

In order to test the computational correctness of the second version of the coded algorithm [EPFM & PCD], three nonlinear mathematical problems are considered. These problems can be stated as:

Table 5.1 Comparison of results for test problem (HJ method)

Obtained by	x_1	x_2	Δx_1	Δx_2	F'_1
Kuester & Mize	0.20576	0.47978	0.00009766	0.00009766	-3873.92355
Present study	0.20566	0.47988	0.00009766	0.00009766	-3873.92355

Problem 1:

$$\text{Minimize} \quad F'_2 = 2\,x^2 + \frac{16}{x} \tag{5.2}$$

subjected to:

$$x \geq 1 \tag{5.3}$$

$$x \leq 5 \tag{5.4}$$

Problem 2:

$$\text{Minimize} \quad F'_3 = 4\,x_1^2 + 3\,x_2^2 - 4\,x_1\,x_2 + x_1 \tag{5.5}$$

Problem 3:

$$\text{Minimize} \quad F'_4 = 2\,x_1^3 + 4\,x_1\,x_2^3 - 10\,x_1\,x_2 + x_2^2 \tag{5.6}$$

Fig. 5.1 shows the variation of the objective function with the decision variable(s) for (a) Problem 1, (b) Problem 2, and (c) Problem 3. To solve these problems, necessary minor modifications are made in the code. The values of ε_{1dv} and ε_{1df} are assumed 3×10^{-5} and 3×10^{-6} respectively for Problem 1. For Problems 2 and 3, the values of ε_{1dv}, ε_{1df} and ntermi are assumed respectively 3×10^{-4}, 3×10^{-4} and 4 respectively. The initial values of ξ and $d\xi$ are respectively 1.0 and 1.0 for Problem 1, and 0.5 and 0.25 for Problems 2 and 3. The search is started with the initial guess of 1 for x in Problem 1, zero for both decision variables, x_1 and x_2 in Problem 2, and 5 and 2 for the decision variables x_1 and x_2

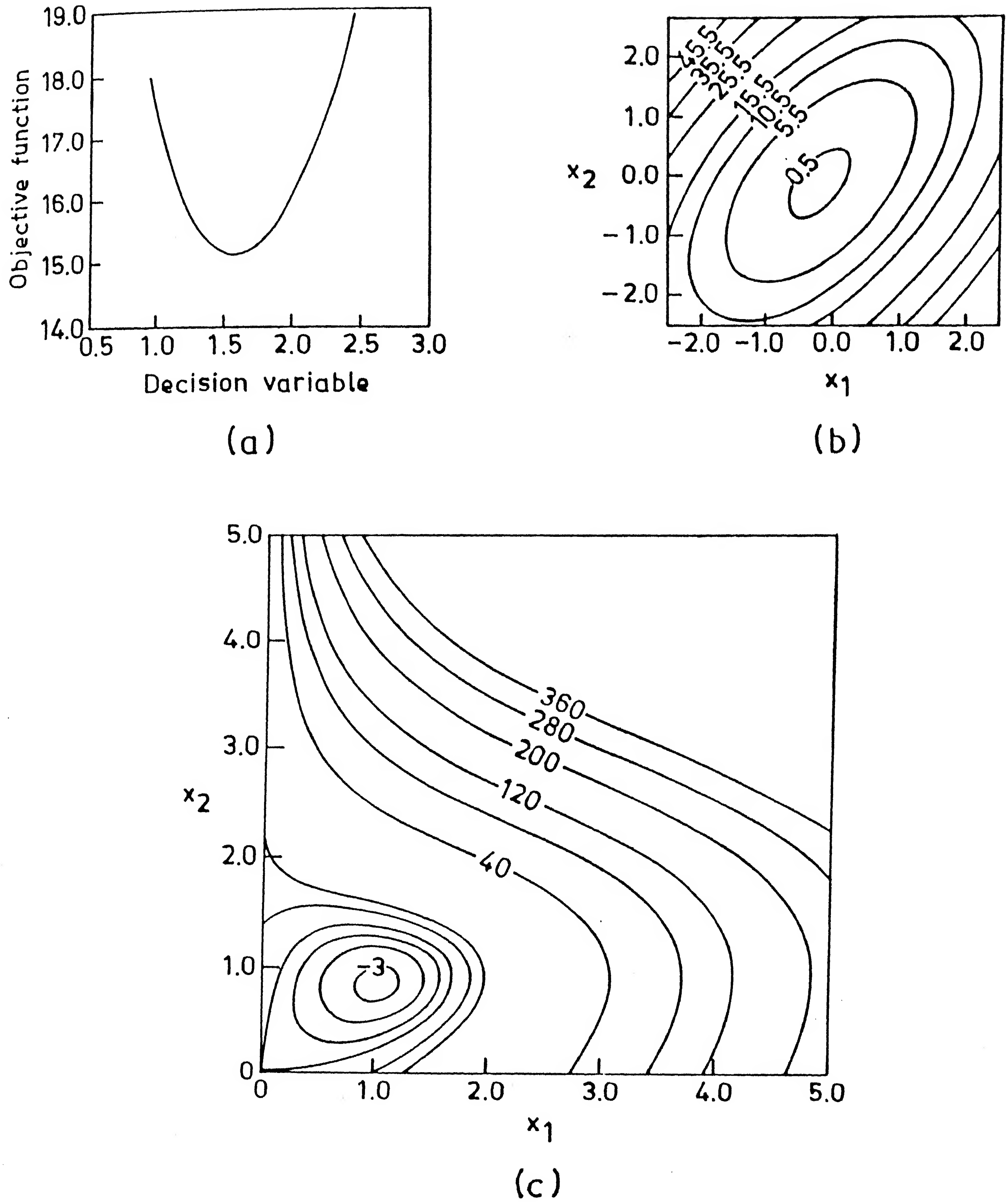


Fig. 5.1 Variation of objective function with decision variable(s) for (a) Problem 1 (b) Problem 2 (c) Problem 3.

respectively. The search direction vector, 'e' to initiate the search process is assumed to be an unit matrix for all problems.

The optimal values of objective functions and decision variables of these three test problems are given in Table 5.2. The exact solutions of these three problems are also presented in this table for comparison. This comparison (Table 5.2) seems satisfactory in establishing the correctness of the optimization code developed. A few other test problems are also evaluated with satisfactory results.

5.2 PERFORMANCE EVALUATION OF GROUNDWATER MANAGEMENT MODELS

To evaluate and assess the performance of the groundwater management models and the algorithms for its solution, Model I is applied to specified study areas with known aquifer parameter values, initial and boundary conditions, and specified aquifer states in context of quality. Model I which is a maximization problem, is solved for the two cases: (A) when a conservative pollutant exists in the aquifer domain, and (B) when no pollutant exists in the aquifer domain or quality aspect is either unimportant or ignored. To assess the performance of the methodology, effect of discretization and sensitivity of the objective function to penalty parameter and initial guesses are described in the following sections. The solution results reported in this section are obtained using exterior penalty function method in conjunction with modified Hooke-Jeeves algorithm. All computations reported in this section

Table 5.2 Comparison of results for test problems (PCD method)

Problem No.	Present study			Exact solution		
	F'	x_1	x_2	F'	x_1	x_2
1	15.11905	1.58742	—	15.11905	1.58740	—
2	-0.09375	-0.18750	-0.12500	-0.09375	-0.18750	-0.12500
3	-3.32409	1.00155	0.83345	-2.86000*	1.00600*	1.07000*

* reported by Reklaitis et al. (1983)

are performed on a Convex/C-220 mini super computer system. The order of violation represents the product of a fractional number (<1) and the value reported in the solution results.

5.2.1 Description of the study area

Fig. 5.2 shows a finite difference network for the study area of 900 ha (3 km x 3 km) divided into square cells, each of size 0.5 km x 0.5 km with Dirichlet boundary condition. The management problem involving both quality and quantity aspects (Case A) is solved for this study area. The aquifer is assumed homogeneous and anisotropic. The hydraulic conductivities K_{xx} and K_{yy} are 5.0×10^{-4} m/s and 4.0×10^{-4} m/s respectively. The storage coefficient, effective porosity, thickness of leaky layer, saturated thickness of confined aquifer, hydraulic head in source bed and ground surface elevation are respectively 2.0×10^{-4}, 0.3, 2.0 m, 30.0 m, 55.0 m, and 62.0 m. These values do not change with respect to space and time. The vertical hydraulic conductivity of overlying leaky layer is 1.0×10^{-12} m/s. The vertical point recharge due to waste injection or some other activity in all the cells except boundary cells is assumed 1.0 l/s throughout the management period. The recharge at all boundary cells is assumed zero. The concentration of chloride entering the internal cells denoted by A and B (Fig. 5.2) are respectively 1000 mg/l and 500 mg/l in recharge, and 200 mg/l and 400 mg/l in leakage. The longitudinal and transverse dispersivities are 30 m and 10 m respectively. The time frames

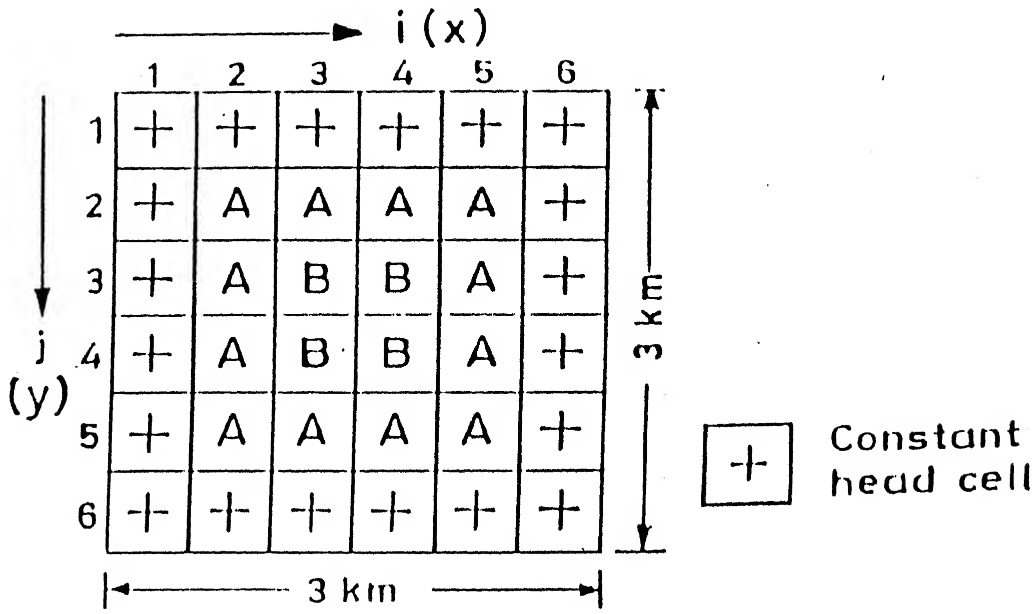


Fig. 5.2 Finite difference network (Case A).

considered in a time horizon of five years are five for all optimization runs except those where stated explicitly.

Fig. 5.3 shows a finite difference network for the study area of 2500 ha (5 km x 5 km) divided into square cells, each of size 0.5 km x 0.5 km with Dirichlet boundary condition. The management problem involving only quantity aspect (Case B) is solved for this study area. The aquifer properties and the values of other parameters remain same except that there is no leakage and recharge in this case. Ten time frames are considered in a time horizon of five years for all optimization runs except those where stated explicitly.

In the top layer of boundary cells (Figs. 5.2 and 5.3), the hydraulic heads are specified as 50.0 m. In the bottom layer of boundary cells, the hydraulic heads are specified as 41.0 m. For the remaining cells, simple interpolation is used to obtain the hydraulic head distribution in the aquifer domain. This distribution is assumed as the specified initial hydraulic heads. Existing concentrations at all boundary cells as required for Case a are specified as 100 mg/l. The initial concentration in the aquifer for the cells denoted by A and B (Fig. 5.2) are 2000 mg/l and 50 mg/l respectively.

The model is subjected to inbuilt lower bounds on hydraulic head, pumping and concentration variables. The spatial and temporal distribution of inbuilt lower bound on hydraulic head is such that the aquifer does not become unconfined anywhere in the aquifer

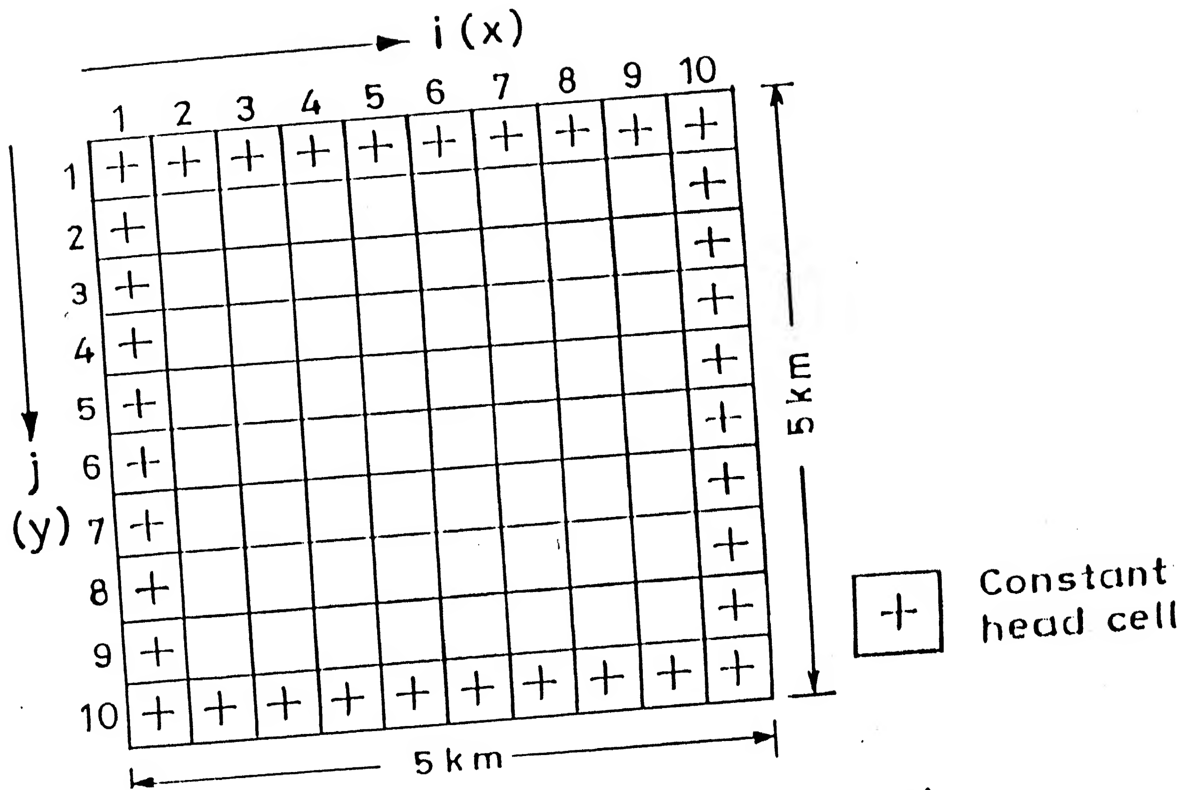


Fig. 5.3 Finite difference network (Case B).

domain. The inbuilt lower bounds on pumping and concentration variables are simply zero to avoid the nonpositive values of these decision variables in space and time. The inbuilt upper bound on hydraulic head represents the ground surface so that area under investigation does not become water logged. There is no inbuilt upper bound on pumping and concentration in space and time.

5.2.2 Effect of time step

To assess the effect of time discretization on the solution of the model, the model is solved for both the Cases A and B with two different time steps. These two time steps are 365 days in first optimization run and 182.5 days in second optimization run. The optimization parameters used for the computation are $r = 10^{-18}$, $\alpha_h = \alpha_q = \alpha_c = 2$ and $\beta_h = \beta_q = \beta_c = 1$. The values of ε_h, ε_q and ε_c used in the runs are 0.001 m, 0.01 l/s and 0.01 mg/l respectively. Optimization runs are started with 40 m, 50 l/s and 100 mg/l as initial solution for hydraulic head, pumping and concentration variables respectively. The starting step sizes are assumed 0.5 m for hydraulic head, 5 l/s for pumping and 10.0 mg/l for concentration variables. In Case B, values of α_c, β_c, ε_c, and initial guesses and starting step sizes for concentration variables are not required. The optimization runs for this case are initiated with 40 m and 500 l/s as the initial solution for hydraulic head and pumping variables respectively.

The solutions of the model in both cases for both runs are

summarized in Table 5.3. It shows that the objective function value decreases by 1.23% in Case A and 1.43% in Case B, if the time step is reduced from 365 days to 182.5 days. These differences in objective function values are marginal. These results for different time steps show that the performance of the groundwater management models is satisfactory with respect to variations in specified time steps.

5.2.3 Effect of grid size

To assess the effect of space discretization on the solution of the model, the model is solved for both the cases with two different grid sizes. The time step considered is 365 days in Case A and 182.5 days in Case B. In the first optimization run, the grid (cell) size is assumed 0.5 km x 0.5 km, whereas in second optimization run, it is assumed 1.0 km x 1.0 km. Two different grid sizes are chosen such that pumping area remains same. In both optimization runs of Case A, the recharge per unit area is kept constant. The pollutant concentration entering the internal cells through recharge and leakage in this case are assumed 750 mg/l and 300 mg/l respectively in the entire aquifer domain, throughout the planning period. The initial pollutant concentration in this case is assumed 1025 mg/l in the entire aquifer domain. These changes in the aquifer environment are made to facilitate the comparison for the study of the effect of space discretization only. The values of optimization parameters, and initial and final step sizes remain same as mentioned in section

Table 5.3 Effect of time step

Case	Run No.	Time step (Day)	Order of violation of simulation constraints (in S.I. unit) FLOW	TRANSPORT	Objective function value (litre)
A	1	365.0	$10^{-9}-10^{-14}$	$10^{-9}-10^{-13}$	1.8109×10^{14}
A	2	182.5	$10^{-9}-10^{-14}$	$10^{-9}-10^{-12}$	1.7886×10^{14}
B	1	365.0	$10^{-9}-0.0$	—	6.2148×10^{14}
B	2	182.5	$10^{-9}-0.0$	—	6.1256×10^{14}

5.2.2. In Case A, run 1 is started with 1250 l/s for pumping, 40 m for hydraulic head and 100 mg/l for concentration variables as initial solution of the model. Run 2 is also started with the same values as initial guesses except that pumping values are taken such that pumping per unit area remains same. Likewise in Case B, run 1 is started with values of 125 l/s for pumping and 40 m for hydraulic head variables respectively as an initial solution of the model. Run 2 is also started with the same values as these initial guesses except that pumping values are taken such that pumping per unit area remains same. This is necessary to have equal hydraulic loading on the aquifer domain to facilitate the comparison.

The optimal solutions of the model in both the cases for both the runs are summarized in Table 5.4. The comparison between the two optimization runs shows that the objective function value does not vary appreciably in both the cases. The objective function value decreases by 12.58% in Case A and 12.44% in Case B if the size of the cell is increased from 0.50 km x 0.5 km to 1.0 km x 1.0 km. This difference occurs because of slight variations in the initial velocity field. In addition, in a coarse mesh, Courant number becomes less than 0.5 and thus, approximation of partial differential equations may involve some truncation error. It is always better to have finer mesh size. It is observed by numerical experimentation that as the cell size is chosen closer to 0.5 km x 0.5 km, this difference reduces. This discrepancy decreases progressively when the obtained solution approaches global optimum.

Table 5.4 Effect of grid size

Case	Run No.	Grid size (km x km)	Order of violation of simulation constraints (in S.I. unit) FLOW	TRANSPORT	Objective function value (l/s)
A	1	0.5 x 0.5	10^{-9} - 10^{-12}	10^{-8} - 10^{-11}	8585.78
A	2	1.0 x 1.0	10^{-10} - 10^{-12}	10^{-10} - 10^{-12}	7505.32
B	1	0.5 x 0.5	10^{-9} - 0.0	—	12960.25
B	2	1.0 x 1.0	10^{-10} - 0.0	—	11348.50

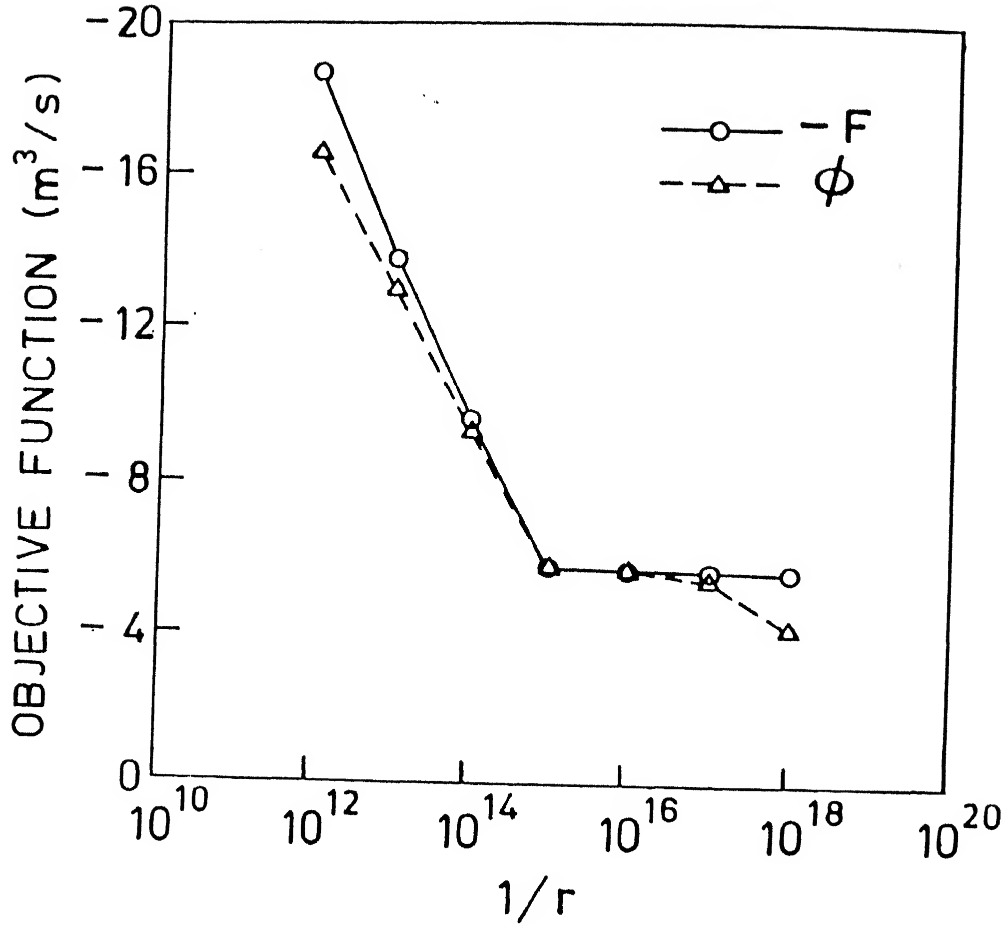


Fig. 5.4 Sensitivity of objective function to penalty parameter.

factors, acceleration factors , termination parameters, initial guesses, and initial step sizes for decision variables as mentioned in section 5.2.2.

It is observed that if r is decreased progressively, even beyond the convergence point, there is no improvement in real objective function (F). the value of composite objective function (ϕ) increases because of the smaller value of penalty parameter. It depicts that beyond the convergence point, better solution can not be obtained for the given set of initial solution. If a very high value of penalty parameter is chosen to start the computation, the unconstrained optimization becomes progressively more difficult to solve, and for certain value of r, computational termination may occur (Fig. 5.5). Therefore, a proper selection of initial value of penalty parameter, and a strategy to update it after each unconstrained search are necessary to avoid the computational breakdown. This phenomena has been discussed in Chapter 3 also. At the time of selection of the initial value of r and a strategy to update its value, it should be kept in mind that values of g_1 and g_2 are always smaller than one in addition to the guidelines discussed in Chapter 3 for the estimation of the penalty parameter.

A satisfactory strategy to update the value of penalty parameter may be to generate a sequence of the parameter values from a geometric series in decreasing order, with a common ratio of 10. The initial value of penalty parameter may be taken in the order of powers of 10, depending upon the order of numerical values of

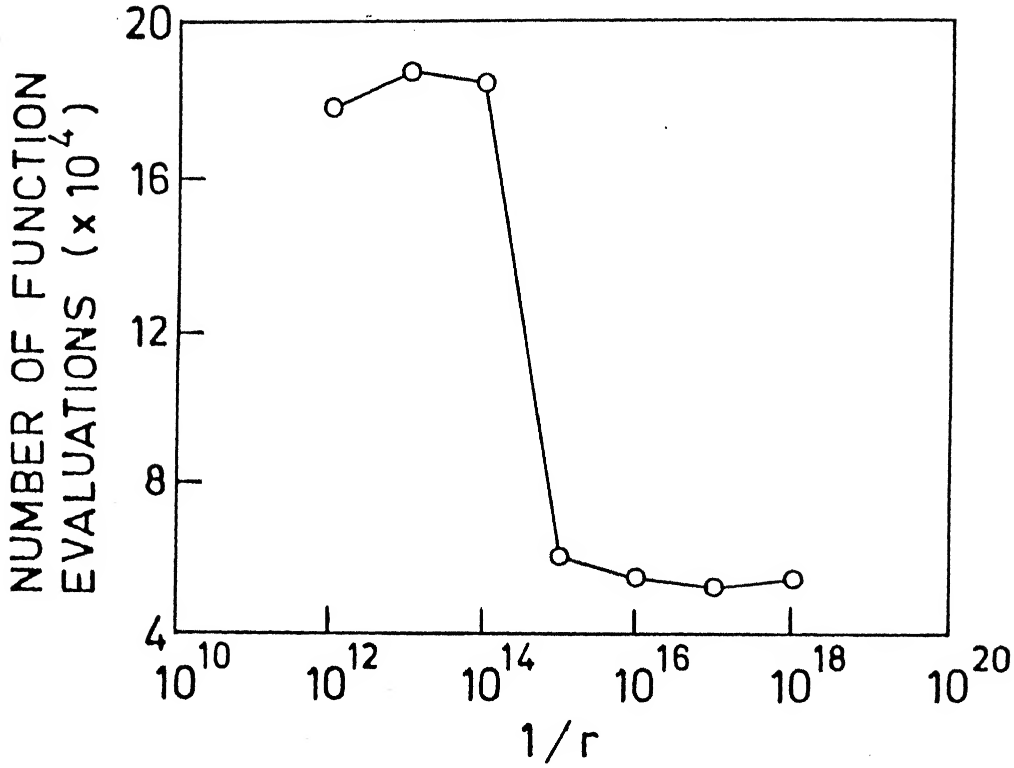


Fig. 5.5 Variation of number of function evaluations with penalty parameter.

objective function and constraints involved in the optimization. It is chosen so as to increase the weight of the constraint violations for exterior forms from stage to stage. However, the variation in penalty parameter value needed to force convergence may cause the resulting unconstrained problem to become progressively ill-conditioned. This is a natural consequence and it can be observed from the distortion occurring in the shape of the contours. This fact has been noted by several investigators, including Murray (1967) and Lootsma (1969). For this particular example problem, it is observed that the initial value of penalty parameter should not be less than 10^{-12}.

5.2.5 Sensitivity of objective function to initial solution

The optimal values of objective and composite objective functions vary with variations in initial guesses for decision variables. However, it is observed that the optimal solution obtained from one set of initial guesses of decision variables can not be improved further even if more iterations are carried out. When the objective function do not improve with additional iterations, a local optimum has been identified. Further, when these local optima do not improve with change in initial guesses also, a global optimum may have been obtained. To establish that the obtained solution is very close to the global optimal, a large number of runs with a large number of initial solution sets are required.

The solutions of the model are obtained with different initial guesses for decision variables to assess the variations in the optimal solutions. The values of reduction factors, acceleration factors, termination parameters, penalty parameter and initial step sizes for decision variables used in the computation remain same as mentioned in section 5.2.2.

Table 5.5 shows the variations in the optimal values of objective and composite objective functions with different initial guesses. It is clear from the table that if the initial guesses for pumping decision variables are increased 10 times, the value of objective function increases by 63.58% and the value of composite objective function decreases by 81.27% for the Case A. However, if the pumping decision variables are again increased 10 times, the values of F and ϕ change marginally. It is evident from the fact that the rate of increase in optimal value of F is only 3.85% and rate of decrease in optimal value of ϕ is only 24.16%. In Case B, the objective function value increases 2.04 times and composite objective function value decreases 12.30 times, if the initial guesses for pumping decision variables are increased 10 times. Further increase in the initial guesses for pumping decision variables by 10 times causes improvement in objective function value by 4.40%, whereas in composite objective function value, it causes depreciation by 39.70%. The results reported here for the Case B account for the vertical leakage into the aquifer through the leaky layer.

Table 5.5 Effect of variation in initial solution on optimal value

Case A				
Initial solution set	Order of violation of simulation constraints		Objective function value	
[h, P, C]	Flow	Transport	F	ϕ
[m, 1/s, mg/1]	(in S.I. unit)		(1/s)	(in S.I. unit)
[40, 50, 100]	10^{-9} - 10^{-14}	10^{-9}-10^{-13}	5736.70	-4.2060
[40, 500, 100]	10^{-10}-10^{-12}	10^{-9}-10^{-12}	9384.02	-7.6200
[40, 5000, 100]	10^{-10}-10^{-11}	10^{-9}-10^{-12}	9745.77	-9.4609

Case B			
Initial solution set	Order of violation of Flow constraints	Objective function value	
[h, P]		F	ϕ
[m, 1/s]	(in S.I. unit)	(1/s)	(in S.I. unit)
[40, 50]	10^{-9}- 10^{-14}	19018.21	-2.2032
[40, 500]	10^{-9} -10^{-12}	33848.49	-27.1098
[40, 5000]	10^{-9} -10^{-12}	40557.89	-19.4056

It shows that optimal solution is very much sensitive to initial guesses. This limitation is however, not unique to the present methodology. This is an inherent limitation of most constrained nonlinear optimization algorithms. To ensure the global optimality of the solution, an exhaustive search for identifying all local optimal solutions are necessary. The detailed discussion on global optimality of management strategies are presented in the following chapter.

5.3 SUMMARY

The constrained nonlinear optimization problems are converted into a sequence of unconstrained nonlinear optimization problems using exterior penalty function method. Thus, validity and applicability of solutions of the groundwater management models rely on the validity and applicability of the unconstrained methods used to solve the models as well as the modeling accuracy. The solutions of some mathematical nonlinear optimization problems using the developed codes and comparison of the solution results with exact solutions appear satisfactory in establishing the validity and accuracy of the implemented optimization algorithms. The groundwater management models dealing with both quantity and quality aspects in an integrated framework, and as a special case, dealing only with quantity aspect are solved using the proposed optimization algorithms. For the study area considered, it is observed that the discretization in space and time does not introduce significant

error. Thus, for different discretization schemes, the difference in optimal values of objective and composite objective functions for different optimization runs are not significant. This conclusion is not valid if modeling requirements represented as restrictions on relevant dimensionless numbers are violated.

The optimal solutions vary with specified penalty parameter and initial guesses for the decision variables. For one set of initial guesses for decision variables, the optimal solution is obtained at the point of convergence. At the point of convergence, the value of objective function and composite objective function (having same nature either maximization or minimization) become almost equal, thus, signifying that order of violation of constraints are negligible at this point. To ensure the global optimality of the solutions, a large number of optimization runs are required, each initiated with different initial solution set. The detailed discussion on global optimality and the impact of physical and managerial constraints on the optimal solutions of different groundwater management models are presented in the next chapter.

RESULTS AND DISCUSSIONS

CHAPTER 6

RESULTS AND DISCUSSIONS

The previous chapter was devoted mainly on the discussions of the performance and validity of the developed groundwater management models, and in particular, that of the implemented optimization algorithms. On the basis of the solutions of some example problems, suitability and applicability of the implemented optimization algorithms were established. The present chapter deals with the performance evaluation of the proposed management models in terms of specific groundwater management problems similar to those encountered in the planning and management of real-world groundwater systems. The impact of various physical, managerial, institutional, political, social, environmental and economic constraints expressed in terms of decision variables explicitly or implicitly, and of natural and man-made activities and/or processes on the optimal solutions of the management models are explored.

Basically, four different groundwater management problems are

considered for these analyses. These problems are: (i) Integrated management for groundwater supply, (ii) Integrated management for groundwater remediation, (iii) Radionuclide pollutant management, and (iv) Special case of groundwater quantity management. The first, third and fourth management problems are based on the Model I (a maximization problem), whereas the second management problem is based on Model II (a minimization problem) as discussed in Chapter 3. The first model (Model I) aims at finding the optimal strategies for groundwater withdrawal to satisfy water demand for various purposes in different aquifer environment and operating situations. The first management problem deals with a conservative pollutant, chloride, whereas the third management problem deals with a radionuclide pollutant, tritium. The fourth management problem is in fact a special case of groundwater extraction management in which only quantity aspect is taken into account. Such situations may occur in those areas where either groundwater pollution is insignificant or quality aspect has no relevance, or assimilative capacity (self purifying capacity) of groundwater system is significant.

The second model (Model II, a minimization problem) aims at finding the optimal policies for the groundwater remediation problem in different operating scenarios. Solution results of various management scenarios designed for each management problem are discussed in details. Most of the solution results are reported with reference to each management period of one year duration within

a larger planning horizon. All computations have been performed on a Convex/C-220 mini super computer with two parallel processors, each having a LINPACK performance of 18 MFLOPS. Solution results reported in this chapter are obtained using exterior penalty function method in conjunction with modified Hooke-Jeeves algorithm.

INTEGRATED MANAGEMENT FOR GROUNDWATER SUPPLY

6.1 INTEGRATED MANAGEMENT FOR GROUNDWATER SUPPLY

Groundwater is withdrawn for various purposes to satisfy the municipal, industrial, agricultural and horticultural demands. In all the cases, supply of desired quantity of water inherently involves the quality aspect. The deterioration of groundwater quality due to natural and man-made activities, industrialization and urbanization, and excessive use of fertilizers for intensive agricultural production has made the quality aspect more significant. In fact, contamination of groundwater has become a serious problem in all industrialized, urbanized and even in rural areas.

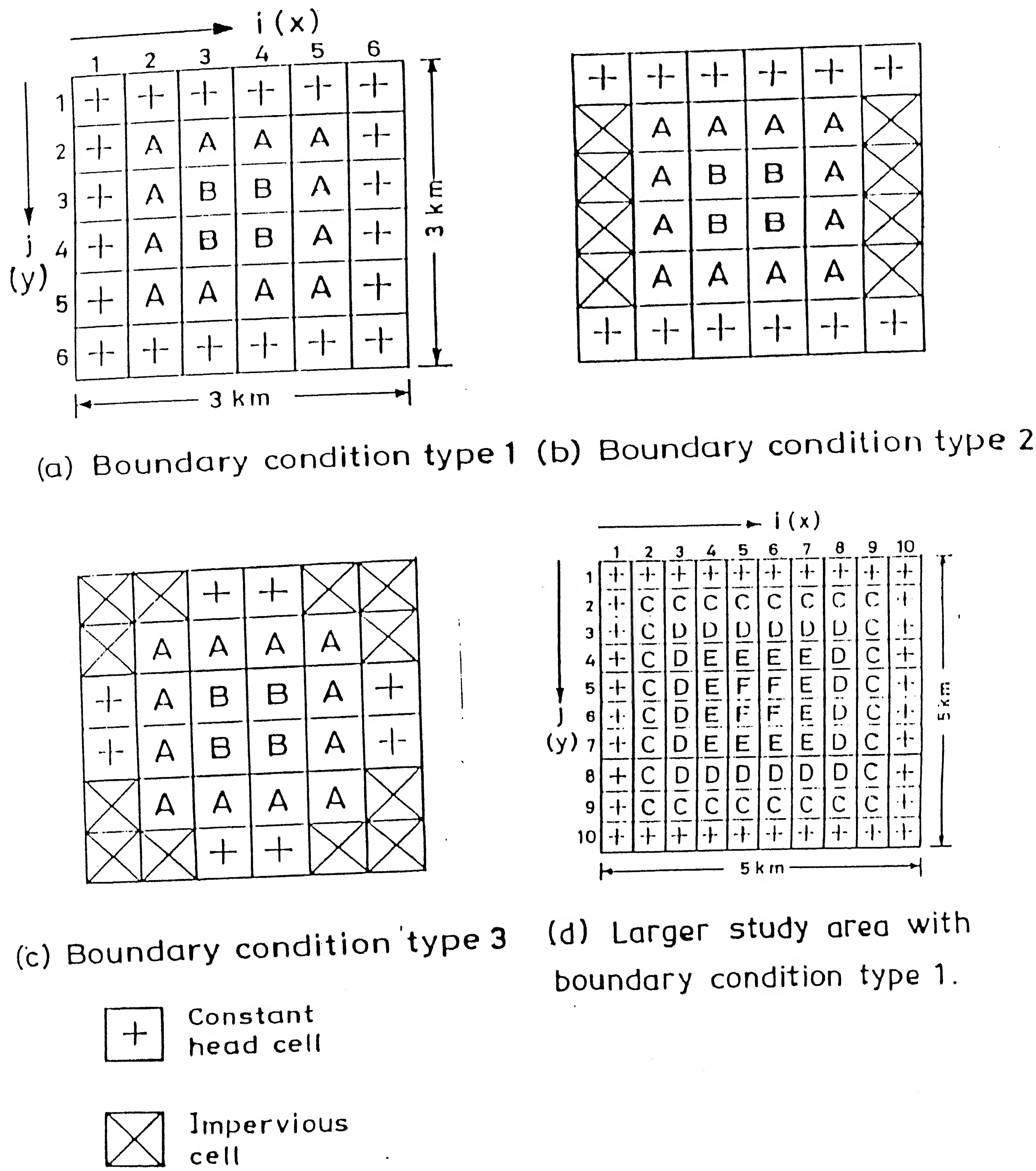
An optimal strategy is needed to cater to the demands of water for specific use with desired quality. To evolve the optimal policies to satisfy the desired demands of water from groundwater resource under imposed restrictions, an integrated management model is developed. The quality and quantity aspects of groundwater are conflated in this model. This model is formulated as a maximization problem (Model I) by embedding the coupled set of discretized flow and transport equations into the optimization model as discussed in Chapter 3. For specific analysis, chloride, a conservative pollutant is considered. The model is applied to specific study areas with known aquifer parameter values, and given initial and boundary conditions. The solution of the model specifies a spatially distributed pumping or withdrawal strategy that optimizes the objective function while meeting all imposed quality, quantity, and other physical and

managerial constraints.

This model is solved for various sets of imposed managerial and physical conditions designated as different management scenarios. The solutions obtained for these scenarios illustrate the variations in the optimal management strategies due to different boundary conditions and variability in aquifer properties. The effects of imposed managerial conditions are also explored. The sensitivity of the optimal value to the variations in the initial guesses for decision variables is also demonstrated. The temporal and spatial variations of hydraulic head, pumping, pollutant concentration and velocity field are also discussed. Effect of leakage through an overlying leaky layer and the effect of pollutant injection are also considered to ascertain the difference in the resulting management strategies.

6.1.1 Description of the study area

Figs. 6.1.1a, 6.1.1b and 6.1.1c show finite difference network for the first study area of 900 ha (3 km x 3 km) with three different physical boundary conditions. Fig. 6.1.1d shows finite difference network for the second study area of 2500 ha (5 km x 5 km) with Dirichlet boundary condition. Both study areas are assumed rectangular divided into square cells, each of size 0.5 km x 0.5 km. To ascertain the qualitative and quantitative aspects of management policies in different aquifer environment and operating conditions, the developed integrated management model is evaluated for a number of



(a) Boundary condition type 1 (b) Boundary condition type 2

(c) Boundary condition type 3 (d) Larger study area with boundary condition type 1.

Fig. 6.1.1 Finite diference network

different scenarios, each depicting different combinations of boundary conditions, managerial constraints, physical situations and aquifer properties. These scenarios are presented in Table 6.1.1.

The aquifer is assumed homogeneous and anisotropic for the management scenarios 1-3 and 8-12. The management scenarios 4, 5 and 6 are based on the assumptions that the aquifer is respectively homogeneous and isotropic, heterogeneous and isotropic, and heterogeneous and anisotropic. To illustrate the effect of heterogeneities and anisotropy, the variations of hydraulic conductivities are assumed exponential. However, the variations of hydraulic conductivities may be approximated by some other deterministic relations such as polynomial, logarithmic, Fourier series, power series etc. or random variations following some well known probability density function (p.d.f.) or stochastic processes. The actual variations of hydraulic conductivities depend upon the best aquifer parameter estimates from the available data. Thus, for illustrative purpose, hydraulic conductivities for the scenarios 5 and 6 are estimated using exponentially varying deterministic expressions of the form:

$$K_{xx} = K_o(1 + e^{a_{xx}x} + e^{a_{xy}y}) \tag{6.1}$$

$$K_{yy} = K_o(1 + e^{a_{yx}x} + e^{a_{yy}y}) \tag{6.2}$$

Where K_o represents the order of hydraulic conductivity of the aquifer domain under consideration. a_{xx}, a_{xy}, a_{yx} and a_{yy} represent

Table 6.1.1 Description of management scenarios (Conservative pollutant)

Management Scenario	Type of Boundary Condition	Hydraulic Conductivity (m/sec) K_{xx}	K_{yy}	Leakage	Recharge	Lower Bounds on $\underline{h}$	$\underline{P}$	$\underline{C}$	Upper Bounds on $\underline{h}$	$\underline{P}$	$\underline{C}$
1	1	5×10^{-4}	4×10^{-4}	y	y	i	i	i	i	n	n
2	2	5×10^{-4}	4×10^{-4}	y	y	i	i	i	i	n	n
3	3	5×10^{-4}	4×10^{-4}	y	y	i	i	i	i	n	n
4	1	4.5×10^{-4}	4.5×10^{-4}	y	y	i	i	i	i	n	n
5	1	HEI		y	y	i	i	i	i	n	n
6	1	HEA		y	y	i	i	i	i	n	n
7	1	Random HEA		y	y	i	i	i	i	n	n
8	1	5×10^{-4}	4×10^{-4}	n	n	i	i	i	i	n	n
9	1	5×10^{-4}	4×10^{-4}	y	y	i	y	i	i	y	y
10	1	5×10^{-4}	4×10^{-4}	y	y	y	y	i	i	y	y
11*	1	5×10^{-4}	4×10^{-4}	y	y	i	i	i	i	n	n
12*	1	5×10^{-4}	4×10^{-4}	y	y	i	y	i	i	y	y

y exists
n does not exist
i inbuilt bound exists

HEI heterogeneous and isotropic
HEA heterogeneous and anisotropic
* For larger study area (10 km x 10 km)

the exponential aquifer parameters which account for the effects of heterogeneity and anisotropy. The first suffix of these quantities signify whether it is used to define K_{xx} or K_{yy}, and the second suffix denotes the direction along which spatial variation in hydraulic conductivity is to be estimated. Thus a_{xx} represents the parameter used in the computation of K_{xx} to account for the spatial variation of K_{xx} in x-direction.

The values of K_o, a_{xx} (= a_{yx}) and a_{xy} (= a_{yy}) for scenario 5 are assumed 10^{-4} m/s, 0.395 km^{-1} and 0.295 km^{-1} respectively. The relative error in the mean value of computed hydraulic conductivities in this case is 0.43%. For the scenario 6, the values of K_o, a_{xx}, a_{xy}, a_{yx} and a_{yy} are assumed 10^{-4} m/s, 0.45 km^{-1}, 0.4 km^{-1}, 0.3 km^{-1} and 0.2 km^{-1} respectively. The relative errors in the mean values of computed K_{xx} and K_{yy} in this case are 0.85% and 0.25% respectively. Heterogeneous and anisotropic characteristic of the aquifer is also modeled using randomly generated spatial values of hydraulic conductivity (scenario 7). In this scenario, the hydraulic conductivity is assumed randomly distributed in space following a Gaussian distribution with standard deviation of 20% of the mean. This mean value is 5×10^{-4} m/s for K_{xx} and 4×10^{-4} m/s for K_{yy}. The relative errors in the mean values of computed hydraulic conductivities in this case are 0.85% for K_{xx} and 1.35% for K_{yy}.

The storage coefficient, effective porosity, thickness of leaky layer, saturated thickness of confined aquifer, hydraulic head in source bed and ground surface elevation are respectively 2.0×10^{-4},

0.3, 2.0 m, 30.0 m, 55.0 m, and 62.0 m. These values do not change with respect to space and time. However, the developed code (NLOGM) can also incorporate spatial variations of these quantities. The model even accounts for the temporal variations of saturated thickness of confined aquifer if it occurs at any location because of subsidence, overstressing, or some other phenomena. The vertical hydraulic conductivity of overlying leaky layer is 1.0×10^{-12} m/s in all the management scenarios where leakage exists. The vertical point recharge when applicable, due to waste injection or some other activity in all the cells except boundary cells is 1.0 l/s throughout the management period. The recharge at all boundary cells is assumed zero. The solute considered here is chloride, a conservative pollutant. The concentration of chloride entering the internal cells denoted by A and B (Figs. 6.1.1a-6.1.1c) are respectively 1000 mg/l and 500 mg/l in recharge, and 200 mg/l and 400 mg/l in leakage. The chloride concentration entering the internal cells denoted by C, D, E and F (Fig. 6.1.1d) are respectively 1000 mg/l, 800 mg/l, 600 mg/l and 400 mg/l in recharge; and 200 mg/l, 300 mg/l, 400 mg/l and 500 mg/l in leakage. The longitudinal and transverse dispersivities are 30 m and 10 m respectively. Five time frames are considered for the scenarios 1-10, whereas for the scenarios 11 and 12, the number of time frames considered are ten in a time horizon of five years. The solution of the model can be easily extended to longer time horizons and larger number of time steps as required.

In the top layer of boundary cells (Figs. 6.1.1a-6.1.1d), the ydraulic heads are specified as 50.0 m. In the bottom layer of oundary cells, the hydraulic heads are specified as 41.0 m. For the remaining cells, simple interpolation is used to obtain the head distribution. The resulting head distribution is considered as the specified initial heads. Existing concentrations at all boundary cells are specified as 100 mg/l for the first study area and zero for the second study area. The initial concentrations in the aquifer for the cells denoted by A, B, C, D, E and F (Fig. 6.1.1) are 2000 mg/l, 50 mg/l, 2000 mg/l, 1000 mg/l, 500 mg/l and zero respectively.

The model has inbuilt lower and upper bounds on hydraulic heads. These inbuilt bounds represent the top of the confining layer and the ground surface respectively. However, these inbuilt bounds can be made redundant by imposing more constraining managerial lower and upper bounds. The inbuilt lower bounds on hydraulic heads are chosen such that the aquifer does not become unconfined. The inbuilt upper bounds on hydraulic heads are chosen such that the area does not become waterlogged. These inbuilt lower and upper bounds basically represent the technical and environmental constraints respectively.

The minimum acceptable pumping is estimated based on the water demand for particular use. This limiting value, representing lower bound on pumping variables in this study is estimated on the basis of irrigation demand from the groundwater source, taking into account both the planting seasons in India (Kharif and Rabi

seasons). It is computed based on the irrigation requirement assuming average climatic conditions of North India, and that only a percentage of the total area is irrigated. If no such lower bound is specified, the model assumes an inbuilt lower bound of zero. The maximum allowable pumping is based on the capacity of maximum two pumps each of 40 H.P. with assumed efficiency of 65 percent. On the basis of the above consideration, the estimated minimum and maximum allowable limits for pumping from each cell are 15 l/s and 100 l/s respectively throughout the planning period. The lower bound on concentration at each cell is zero, while the upper bound imposed is 250 mg/l for all the management period.

6.1.2 General discussion of results

To obtain the optimal solutions, the optimization runs for different management scenarios are started with initial values of 40.0 m, 50 l/s and 100.0 mg/l for hydraulic head, pumping and concentration variables respectively. The values for ε_h, ε_q and ε_c are taken 0.001 m, 0.01 l/s and 0.01 mg/l respectively. The starting step sizes are assumed 0.5 m for hydraulic head, 5 l/s for pumping and 10.0 mg/l for concentration variables. The optimal solutions of different management scenarios for $r = 10^{-18}$, $\alpha_h = \alpha_q = \alpha_c = 2$ and $\beta_h = \beta_q = \beta_c = 1$ are reported in Table 6.1.2. This table provides the information about required CPU time, order of violation of flow and transport equations, optimal total pumping, optimal value of composite objective function, and number of function evaluations

Table 6.1.2 Solution Results for management scenarios (Conservative pollutant)

Management Scenario	No. of Decision Variables	No. of Simulation Constraints	CPU Time (Min.)	No. of Function Evaluations	Order of Violation of Constraints Flow (Transport) (in S.I. unit)	Optimal Total Pumping for 5-Yr. Planning Period (l/s)	Optimal Value of Composite Objective Function (in S.I. unit)
1	240	160	19.11	54824	$10^{-9}-10^{-14}$ ($10^{-9}-10^{-13}$)	5736.70	-4.2060
2	240	160	25.10	72621	$10^{-9}-10^{-12}$ ($10^{-9}-10^{-13}$)	3810.53	-1.3167
3	240	160	25.83	73583	$10^{-10}-10^{-13}$ ($10^{-9}-10^{-12}$)	3438.59	-3.3480
4	240	160	26.75	76469	$10^{-10}-10^{-13}$ ($10^{-9}-10^{-13}$)	6162.96	-2.3075
5	240	160	19.15	54824	$10^{-10}-10^{-12}$ ($10^{-9}-10^{-12}$)	6777.00	-6.3835
6	240	160	14.81	42318	$10^{-9}-10^{-12}$ ($10^{-8}-10^{-11}$)	5268.80	6.7829
7	240	160	27.21	77912	$10^{-9}-10^{-12}$ ($10^{-9}-10^{-11}$)	5853.11	-0.9007
8	240	160	17.79	50976	$10^{-9}-10^{-12}$ ($10^{-8}-10^{-11}$)	6080.32	6.4494
9	240	160	9.06	25964	$10^{-6}-10^{-14}$ ($10^{-5}-10^{-13}$)	5636.47	2.8702×10^{7}
10	240	160	14.84	42318	$10^{-9}-10^{-12}$ ($10^{-8}-10^{-11}$)	3158.18	2.9932
11	1920	1280	1669.61	702893	$10^{-8}-10^{-13}$ ($10^{-8}-10^{-11}$)	23854.73	375.5582
12	1920	1280	1493.76	626073	$10^{-6}-10^{-12}$ ($10^{-5}-10^{-13}$)	19400.06	3.1656×10^{8}

required to obtain optimal values for different management scenarios. The order of violation represents a magnitude equal to the product of a fractional number (<1) with the values reported in Table 6.1.2. Table 6.1.3 shows the yearly optimal pumping policies from the entire aquifer for different management scenarios.

The management scenarios 11 and 12 demonstrate that the developed methodology can be applied to a larger sized study area for a longer time frame. It demonstrates the applicability, robustness and versatility of Hooke-Jeeves method in conjunction with exterior penalty function method. It is observed that this method is suitable for embedding technique which involves large number of variables and constraints to simulate the system. This investigation shows that even a larger sized study area for a large time span can be solved by using this method. The drawback is that it will take a large CPU time for even a single optimum solution of a dimensionally large problem. The CPU time requirements presented in Table 6.1.2 show that as the number of decision variables are increased 8 times (scenario 1 and scenario 11), the CPU time required to obtain the optimal solution for a particular value of r increases approximately 87 times. However, it is observed that the methodology adopted for the solution of the model guarantees its performance in locating at least a local optimum for any type of groundwater management problems without any computational breakdown. With more advanced computers, the CPU time requirements will also decrease.

The practical application of this methodology will require adv-

Table 6.1.3 Yearly optimal pumping policies for management scenarios (Conservative pollutant)

Management Scenario	Optimal pumping (l/s) in Management period (year)				
	1	2	3	4	5
1	1836.45	937.27	980.13	988.72	994.13
2	769.83	699.93	785.90	742.96	811.90
3	873.32	720.14	613.26	615.74	616.13
4	1855.59	1102.90	1163.71	1090.02	950.74
5	1770.61	1199.42	1264.27	1265.71	1273.97
6	1779.64	854.82	872.04	889.09	873.20
7	1636.32	969.30	927.77	1147.99	1174.75
8	1756.62	1086.67	1084.76	1074.63	1077.64
9	1570.82	1024.47	1013.72	1013.73	1013.73
10	299.39	376.27	1023.71	886.87	571.93
11	8312.36	4376.79	3841.10	3573.84	3750.62
12	5989.98	3567.99	3294.36	3232.40	3315.32

anced computing facility. The large multivariable constrained nonlinear problems can be handled successfully using this methodology on high speed computers. The computer memory requirement for storage is very modest in this particular methodology. Exhaustive investigations for different sets of inputs, under different physical, managerial, other technical and nontechnical constraints did not show any failure of the HJ method in obtaining solutions of the groundwater optimization problems. This observation is valid irrespective of the size of the problem, provided the best estimate of initial value of penalty parameter is taken to avoid premature termination and computational breakdown. However, obtained solution can not be guaranteed to be global optimum one, if it has been obtained with only one set of initial solutions. This is an inherent problem of most constrained nonlinear problems. The problem arises because of nonconvex nature of the mathematical model which is common in most of the engineering applications. It is observed that scaling and sparse constraint matrices do not adversely affect the solution. The scaling problem is moderately eliminated by the modifications implemented in the HJ algorithm as discussed in Chapter 4. The problem of sparse constraint matrices is less likely to occur.

6.1.3 Effects of boundary conditions

The optimal value of objective function depends upon the boundary condition of the groundwater system under consideration. Fig.

6.1.2 shows that transient pumping strategy will be different for different types of boundary conditions. Therefore, it is necessary to model the system precisely, describing the real-world system adequately. Otherwise the obtained optimal solution for pumping schedule will reflect the solution for a different system. It is also observed here that the permissible amount of optimal pumping increases as the number of constant head cells at the boundary increase. Presence of impermeable boundaries cause reduction in the optimal pumping.

Figs. 6.1.3-6.1.5 show the spatial distribution of pollutant concentration in fifth management period for scenarios 1-3 respectively. Due to the initial flow gradient in north to south direction, the pollutant travels towards south (y-direction). However, pumping changes the initial flow field by inducing the flow directions towards the central area of the aquifer domain. It is clearly depicted by the Figs. 6.1.6-6.1.8 which show the direction of the velocity vector existing in fifth year in the aquifer at different locations. It is clearly seen from these figures that in the fifth year, the water movement is towards the centre of the study area and more water is withdrawn from the central area of the aquifer. The heavy polluted water from the outer cells rushes towards this zone and causes increase in the pollutant concentration. But due to heavy withdrawal from the cells located in this zone, the final concentration of pollutant becomes moderate (Figs. 6.1.3-6.1.5). It should be noted from Fig. 6.1.5 that pollutant concentrations at the

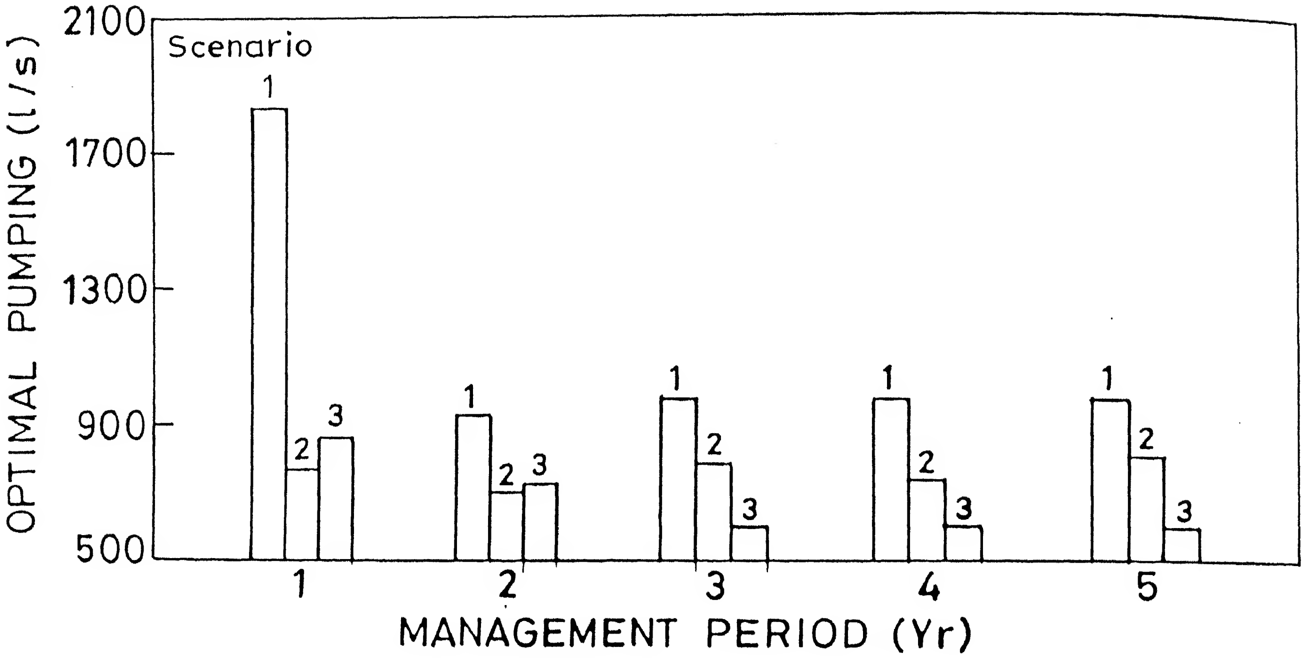


Fig. 6.1.2 Effect of specified boundary conditions on transient optimal pumping.

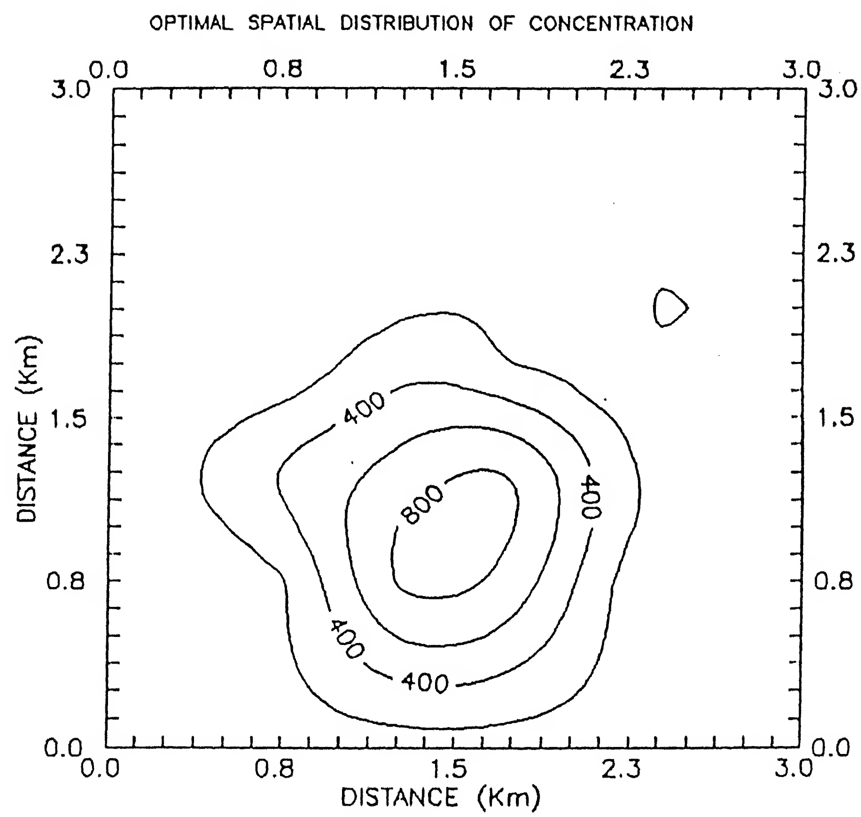


Fig. 6.1.3. Optimal spatial distribution of concentration for scenario 1 in fifth year.

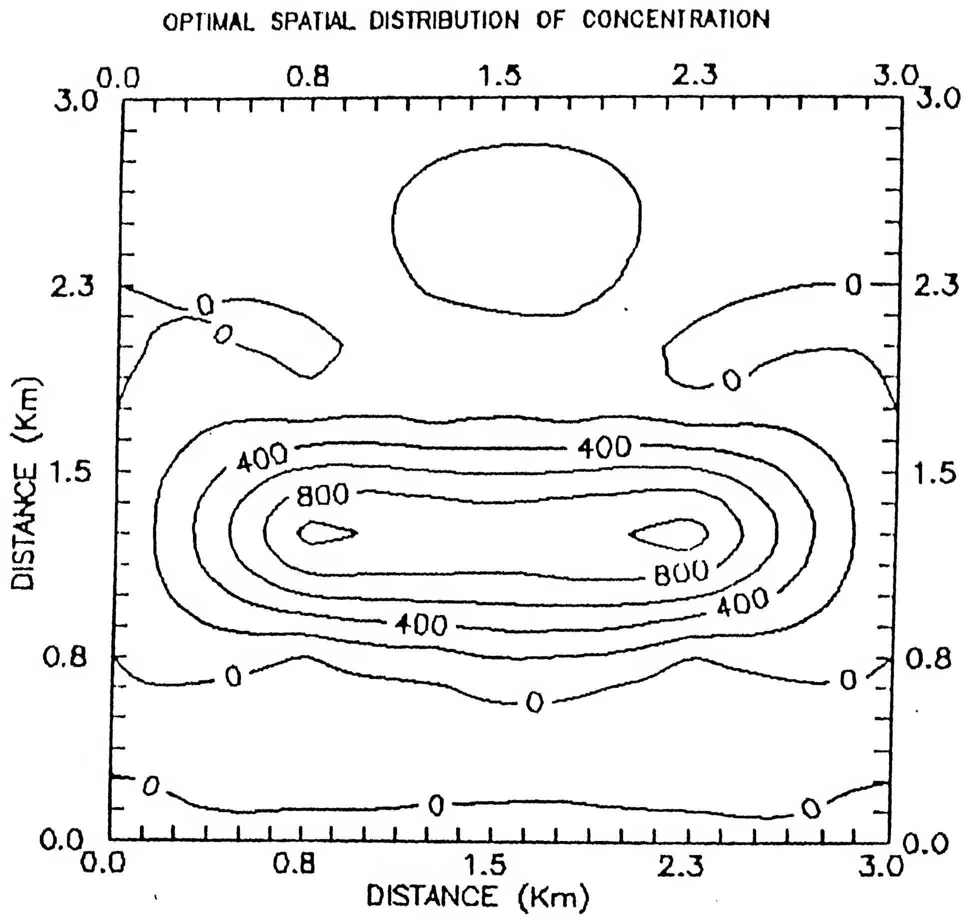


Fig. 6.1.4. Optimal spatial distribution of concentration for scenario 2 in fifth year.

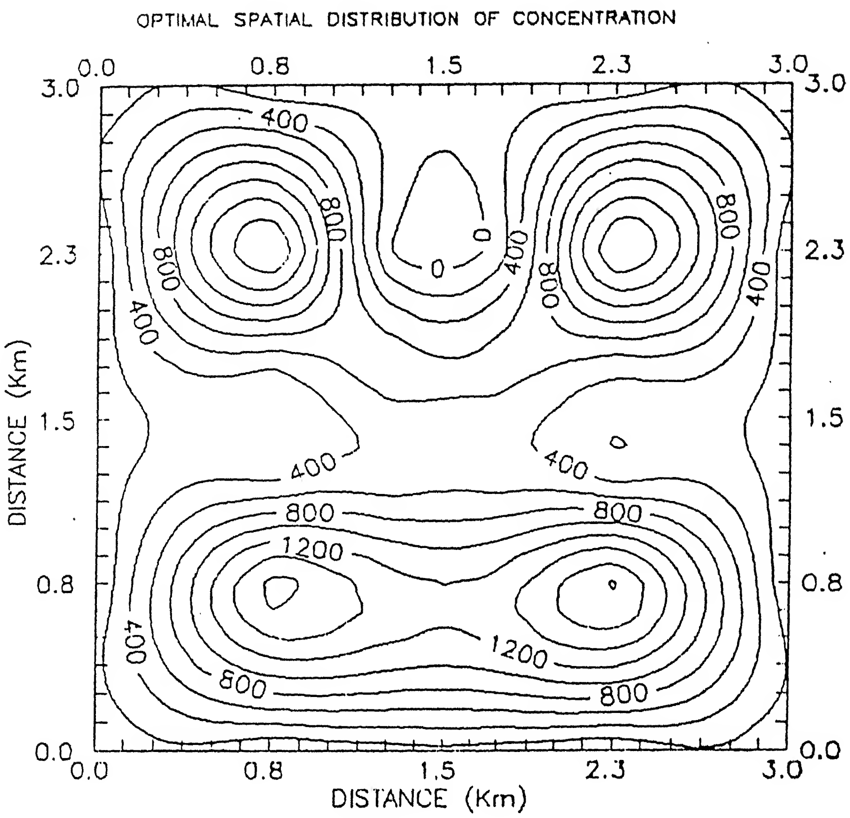


Fig. 6.1.5. Optimal spatial distribution of concentration for scenario 3 in fifth year.

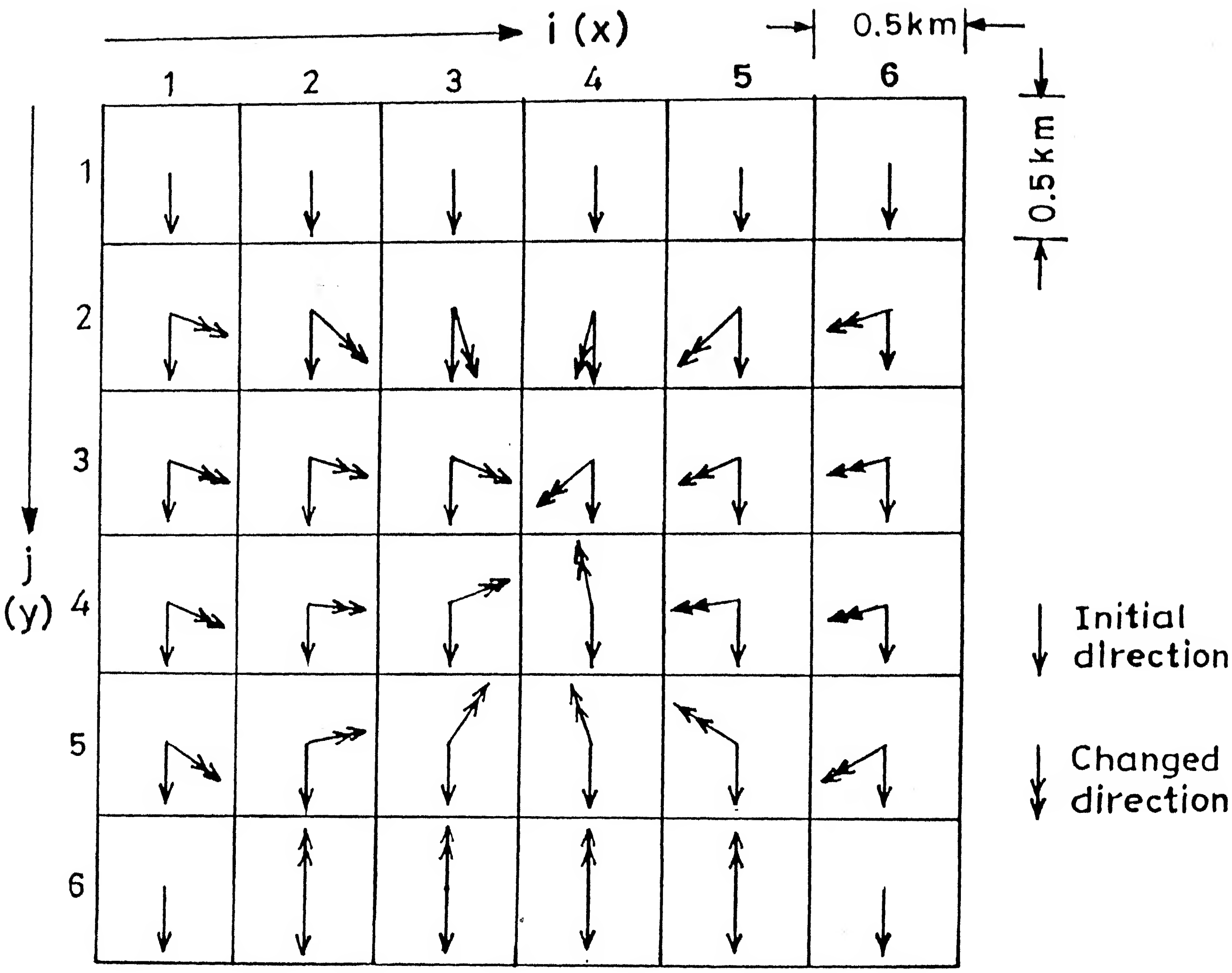


Fig. 6.1.6 velocity field for scenario 1 in fifth year

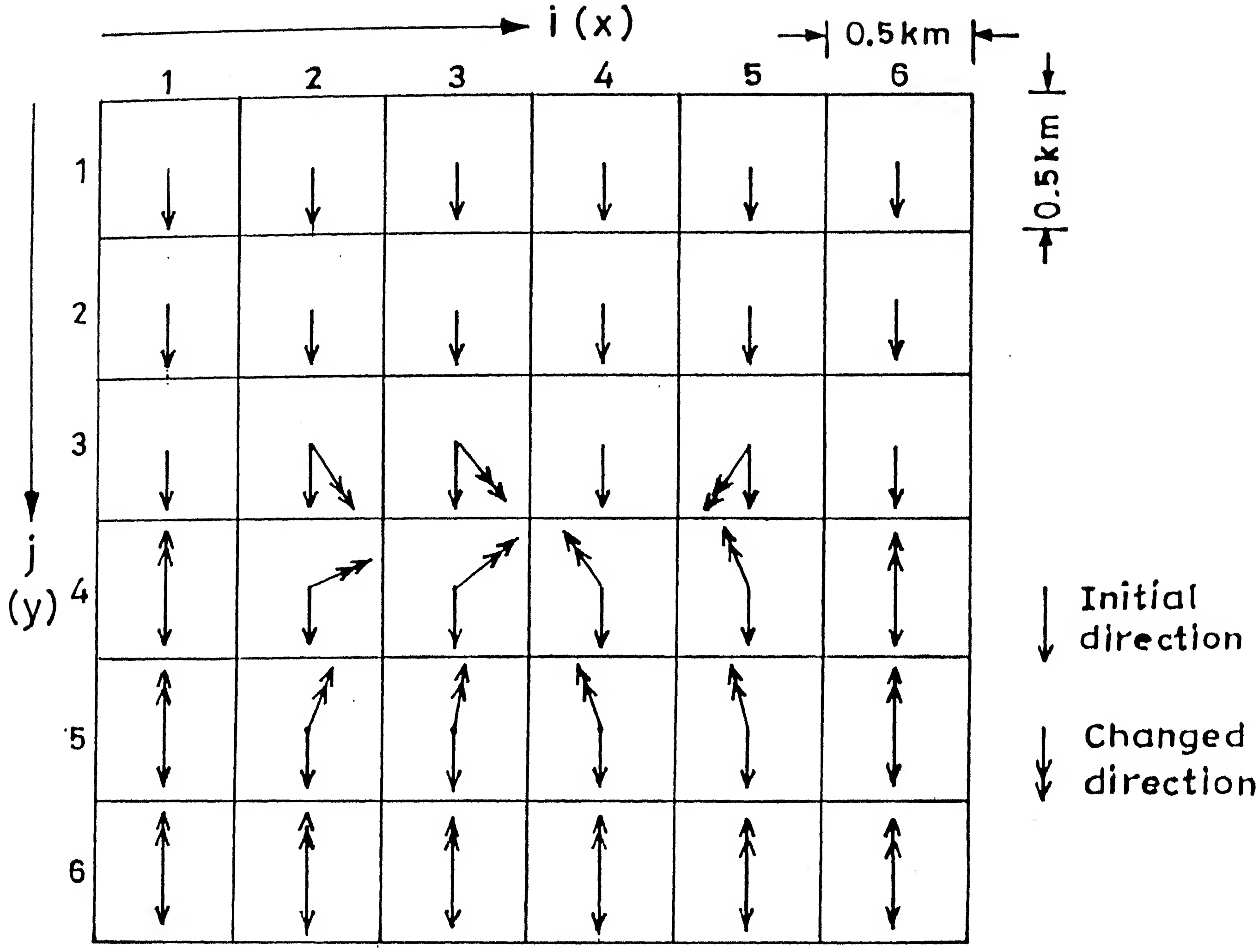


Fig 6.1.7 velocity field for scenario 2 in fifth year

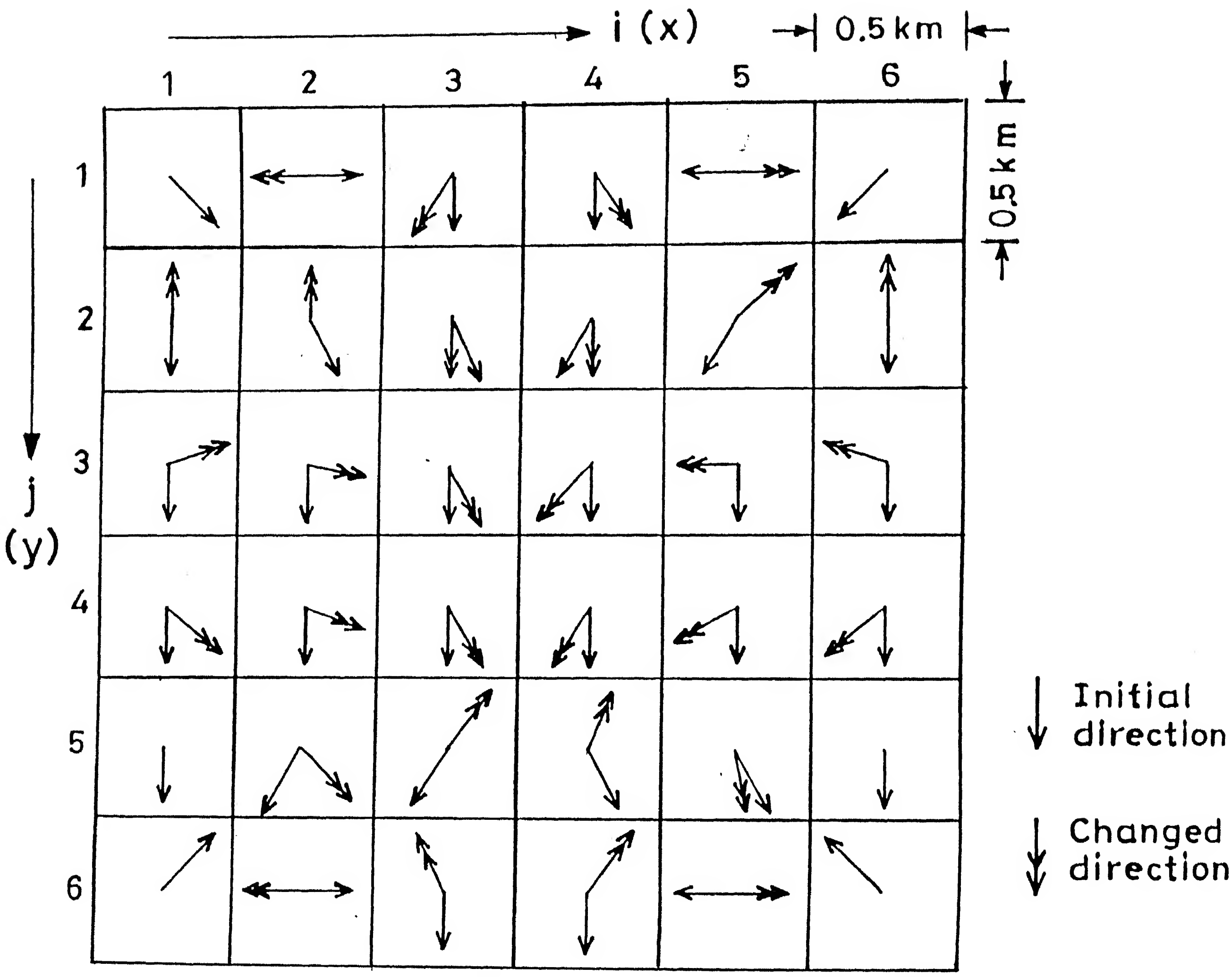


Fig. 6.1.8. velocity field for scenario 3 in fifth year.

corner cells do not reduce appreciably. This is caused by the presence of adjacent impermeable cells. The spatial optimal pumping policies in fifth year of planning for the scenarios 1, 2 and 3 are given in Tables 6.1.4-6.1.6 respectively.

Figs. 6.1.9-6.1.11 show the spatial distribution of hydraulic head in the fifth year of planning for scenarios 1-3 respectively. The distribution is slightly unsymmetrical about y-axis for scenario 2 (Fig. 6.1.10). However, in case of scenario 3, the spatial distribution of hydraulic head is slightly unsymmetrical about both the axes. It should be noted here that some velocity of lesser magnitudes exists along the impermeable boundary. But there is no velocity across the impermeable boundary (Figs. 6.1.10-6.1.11). At the corner cells in case of scenario 3, velocity is of negligible magnitude (Fig. 6.1.11). The velocity along the impervious boundary exists because of the treatment adopted in the modeling for such type of boundary conditions. However, contours get slightly distorted because of this, but it does not affect the solutions appreciably.

6.1.4 Effect of hydraulic head constraints

If the lower bound on hydraulic head is raised, the transient rate of optimal pumping and total pumping for the planning period decrease accordingly. The lower bounds on hydraulic head variables are kept 40 m for first and second years, 35 m for third and fourth years, and 30 m for fifth year in the entire aquifer domain under investigation (scenario 10). The impact of these constraints on

Table 6.1.4 Optimal pumping policy in fifth management period for scenario 1

	Optimal pumping (l/s)			
i →	2	3	4	5
j ↓				
2	81.98	124.00	109.00	72.99
3	41.47	80.50	143.51	39.22
4	32.83	30.02	55.33	112.42
5	13.34	35.88	10.82	10.81

Table 6.1.5 Optimal pumping policy in fifth management period for scenario 2

	Optimal pumping (l/s)			
i →	2	3	4	5
j ↓				
2	100.18	100.34	67.69	78.04
3	0.00	31.44	150.27	51.94
4	0.00	105.69	14.21	0.00
5	0.00	82.58	29.48	0.00

Table 6.1.6 Optimal pumping policy in fifth management period for scenario 3

	Optimal pumping (l/s)			
i →	2	3	4	5
j ↓				
2	1.01	90.54	90.72	14.89
3	48.97	43.00	8.12	50.10
4	48.95	4.00	10.00	29.45
5	0.61	77.81	53.44	44.49

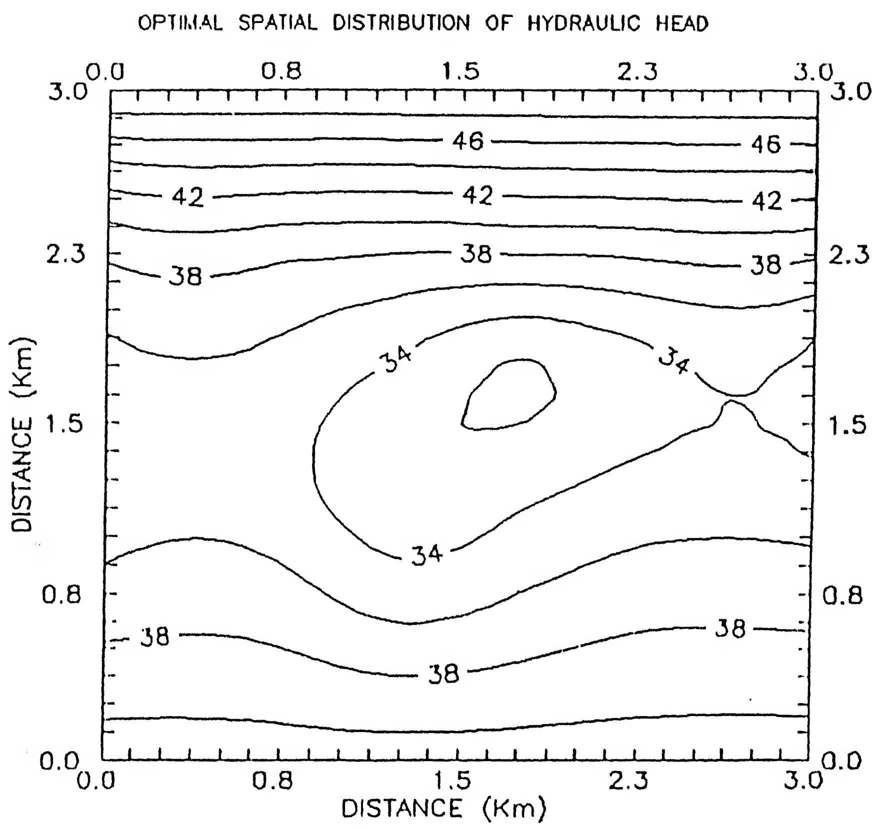


Fig. 6.1.10. Optimal spatial distribution of hydraulic head for scenario 2 in fifth year.

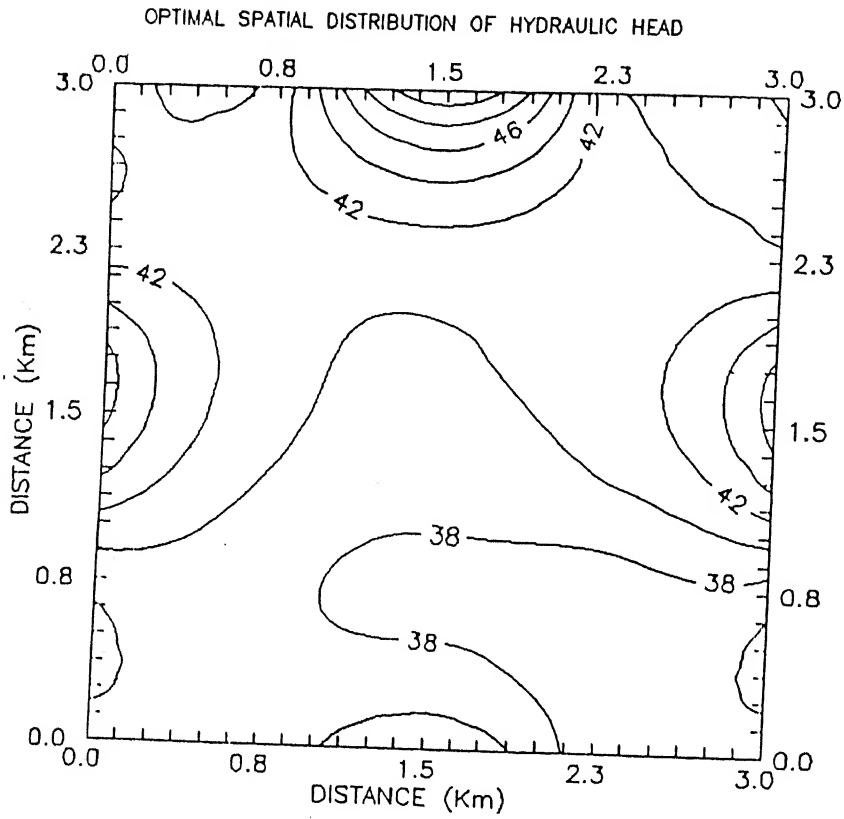


Fig. 6.1.11. Optimal spatial distribution of hydraulic head for scenario 3 in fifth year .

optimal pumping at different time is shown in Fig. 6.1.12. The constraining lower bounds on hydraulic head variables do not allow pumping of more water from the aquifer.

6.1.5 Effect of aquifer parameter estimates

Often a heterogeneous and anisotropic aquifer is modeled for convenience as a homogeneous and isotropic aquifer. Most of the time the reason for such simplified modeling is the nonavailability of spatial aquifer parameter estimates. However, the spatial variation in these parameter values affect the solution of the management model. Therefore, if an aquifer is modeled as homogeneous and isotropic with respect to hydraulic conductivity for example, while in reality the aquifer is heterogeneous and anisotropic, the obtained solutions are strictly applicable to the assumed system and not the real one.

The management policies evolved from a simplified model will involve the risk due to uncertainties in aquifer parameter estimates. In real life situations these parameters vary appreciably. Generally for the modeling purposes, variation in standard deviation of hydraulic conductivity may be taken 5%, 10% and 25% of the mean (Whiffen and Shoemaker, 1993; Latinopoulos et al., 1994). Likewise, the uncertainty in dispersivity is due to large variation of the ratio of longitudinal and transverse dispersivities. This ratio ranges commonly between 3 and 100 (Bear and Verruijt, 1987). Thus, an inadequate and oversimplified model may yield a solution which

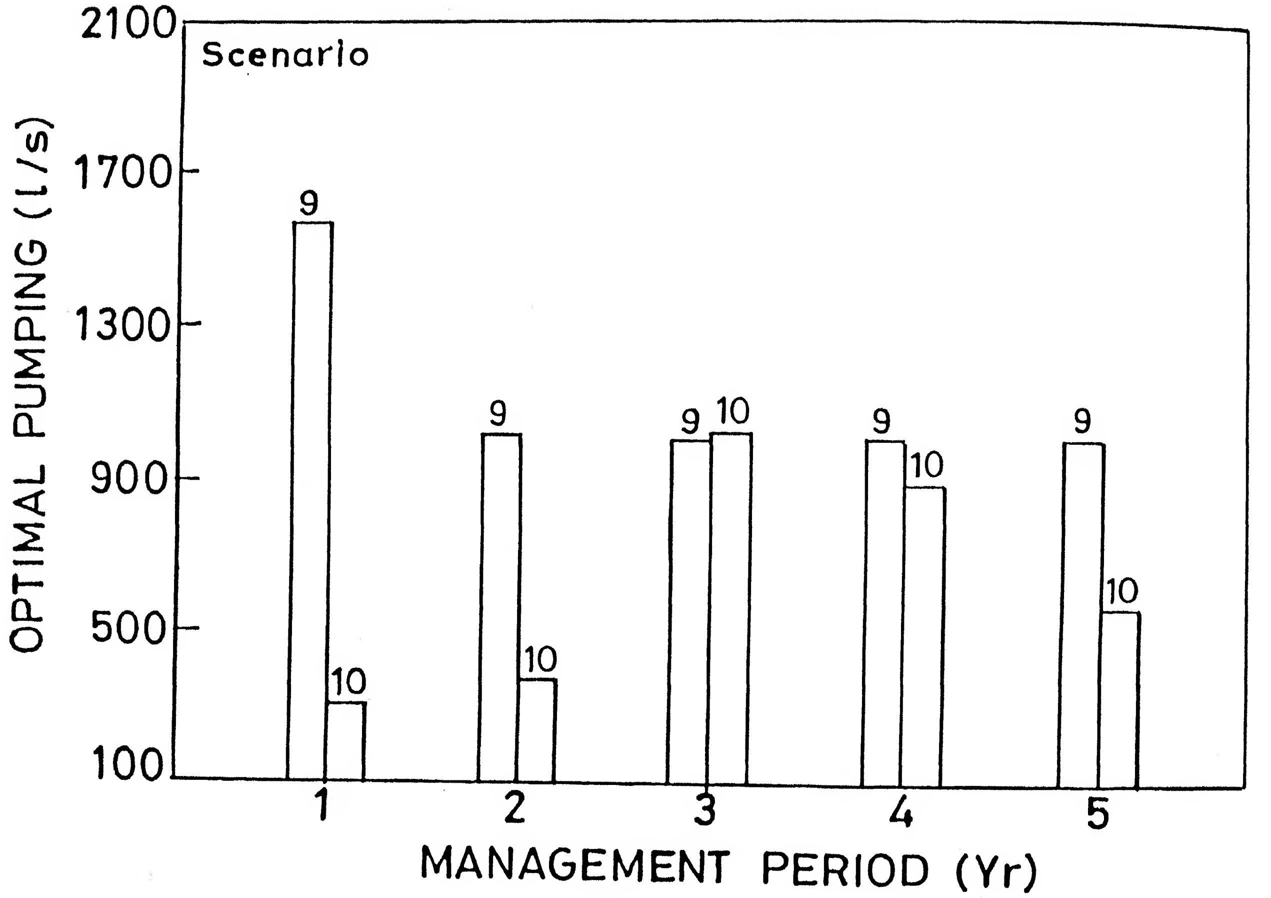


Fig.6.1.12 Effect of hydraulic head constraints on transient optimal pumping.

will not have proper relevance of its objectives. For illustrative purpose, the effect of variability of hydraulic conductivity estimates on the optimal policies is reported here.

The variation in the solution results with and without the simplified assumptions of homogeneity and isotropy are demonstrated in Figs. 6.1.13-6.1.15. Figs. 6.1.13-6.1.14 show the effects of deterministic variations of hydraulic conductivities on the optimal solution, for a few typical cases. Fig. 6.1.15 shows a comparison between optimal solutions for typical deterministic variations and a typical randomized variation following a Gaussian distribution with standard deviation of 20% of the mean. The relative values of the objective functions are not important in these comparisons because, these are only a few illustrative comparisons. These difference in values however, demonstrate the significance of proper parameter estimations. The relative magnitudes can be assessed accurately only when a large number of cases are optimized and global optimum solutions are available.

6.1.6 Effect of natural and man-made activities

If the aquifer is leaky and there is some pollution in the overlying stratum, the pollutant will travel with water and will affect the pollutant concentration in the aquifer. If leakage with high concentration from overlying stratum enters the aquifer, the concentration in the aquifer increases, otherwise it may decrease due to the leakage. Man-made activities such as waste injection also

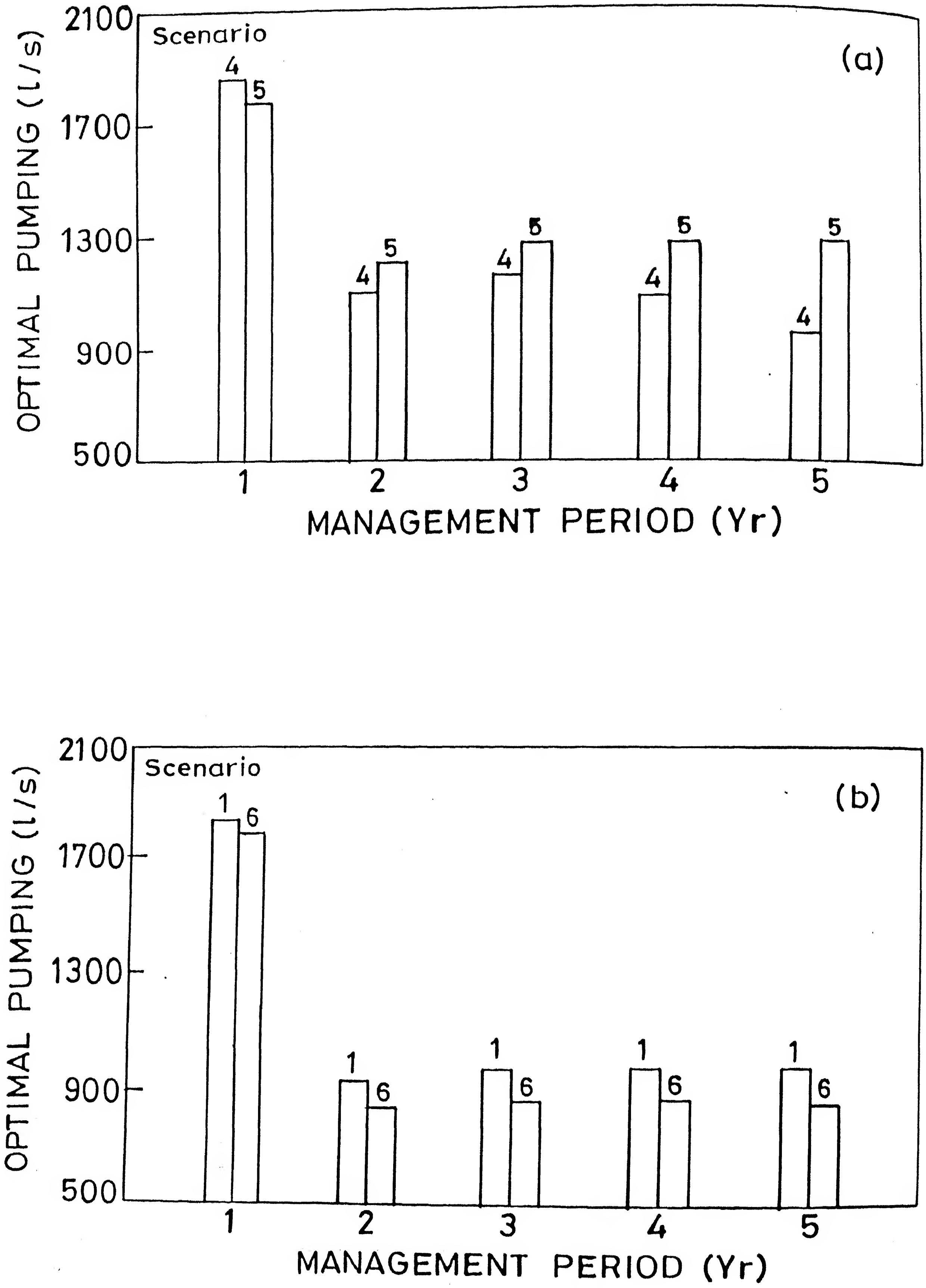


Fig.6.1.13 Effect of heterogeneity on transient optimal pumping from (a) isotropic aquifer (b) anisotropic aquifer.

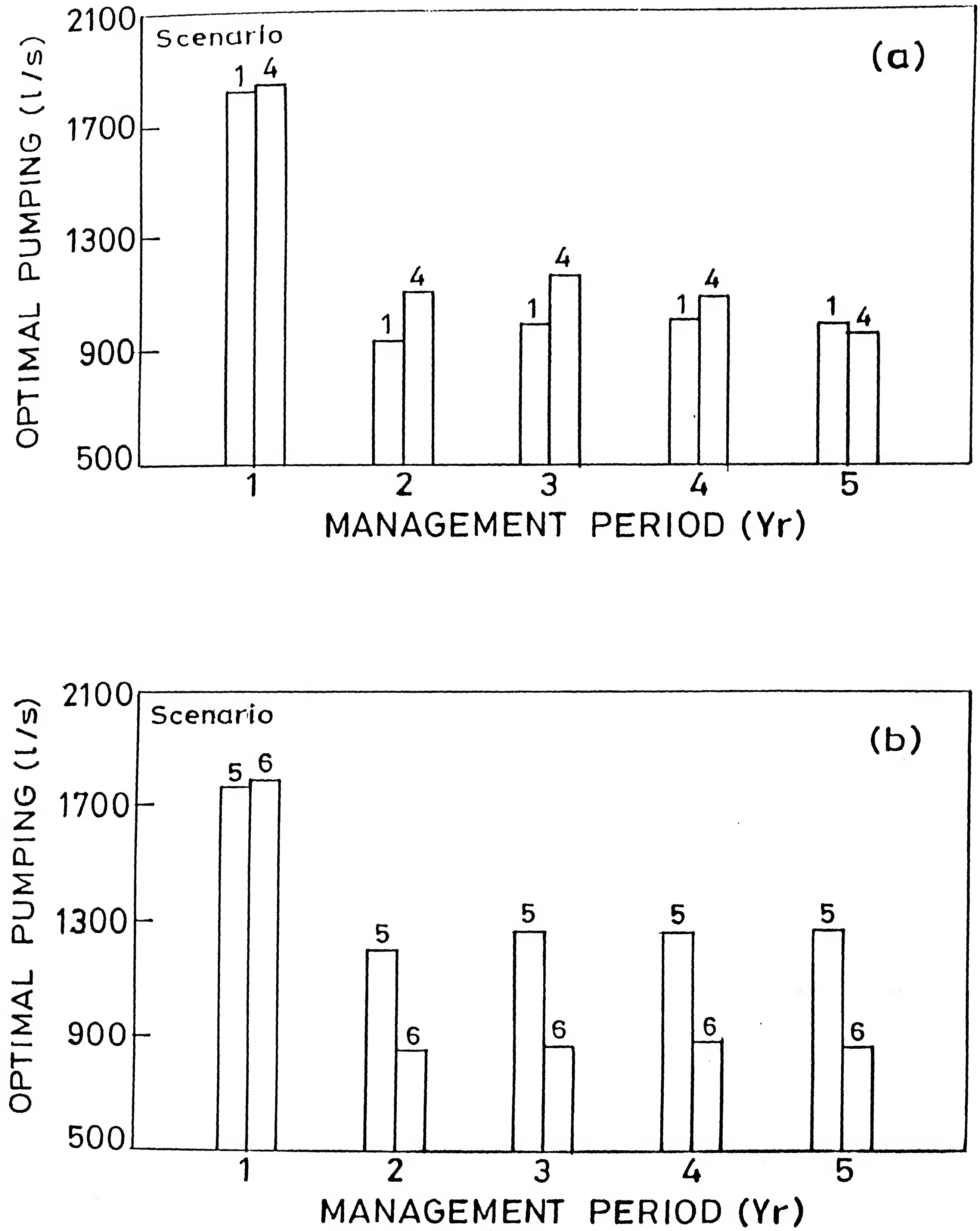


Fig.6.1.14 Effect of anisotropy on transient optimal pumping from (a) homogeneous aquifer (b) heterogeneous aquifer.

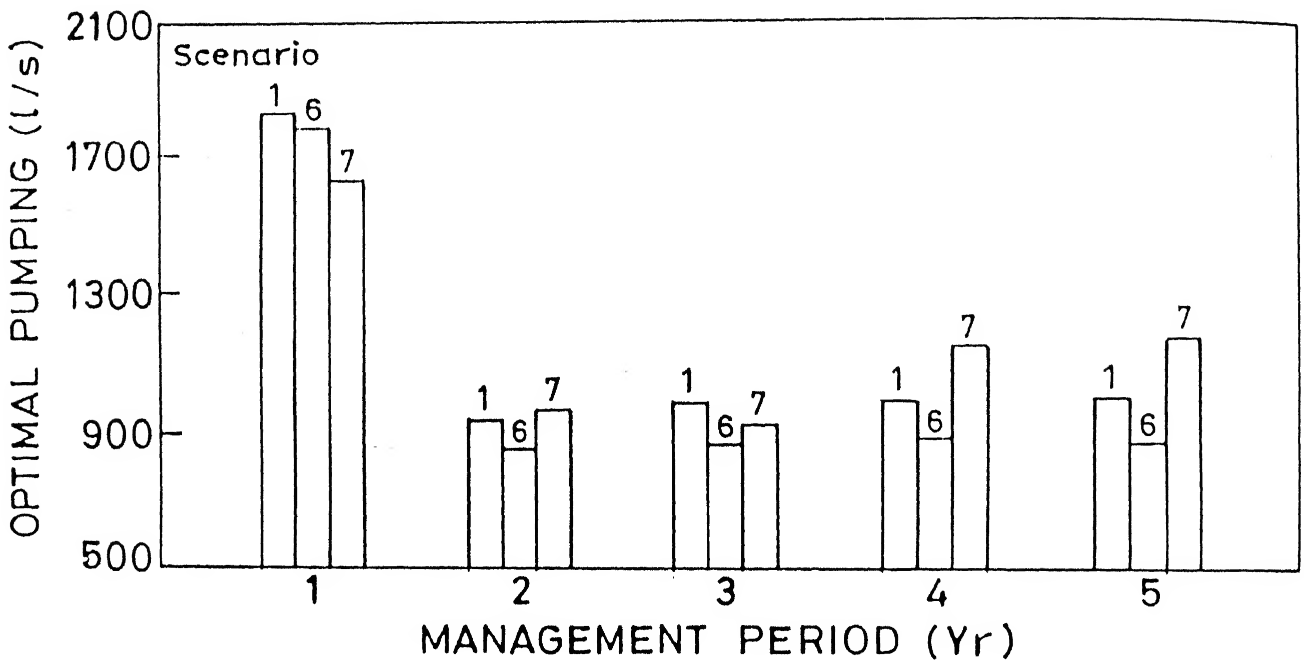


Fig. 6.1.15 **Effect of deterministic and randomized modelling of heterogeneous hydraulic conductivity on transient optimal pumping rates.**

affect the strength of pollutant in the aquifer. In such cases, the optimal pumping schedule will be different from that situation where leakage and recharge by waste injection or some other activities do not exist in the system (Fig. 6.1.16). The results shown in Fig. 6.1.16 can not establish the relative effects of leakage and recharge on optimal pumping schedule. The reason is that these solutions may represent only local optimal solutions, as global optimal cannot be guaranteed. A valid comparison can be done only when the global optima are obtained. The idea behind this presentation is simply to show the significance of the natural and man-made processes that are included in modeling the system. These solutions are also useful for estimating the excitation responses as a result of implementing these optimal policies.

6.1.7 Global optimality of management strategies

The optimal results depend upon the value of penalty parameter as discussed in Chapter 5. The convergence of the optimal values can be obtained for each management scenario by increasing the number of runs with different values of r. The optimal value depends also on the values of α, β and ε. α and β decide the directions of search and move respectively, whereas ε allows more number of iterations to obtain the desired solution. If proper values of α, β and ε are not used, the directions of search and move during the minimization process may change in such a way that solution is achieved because of premature termination. It can not be guaranteed that obtained

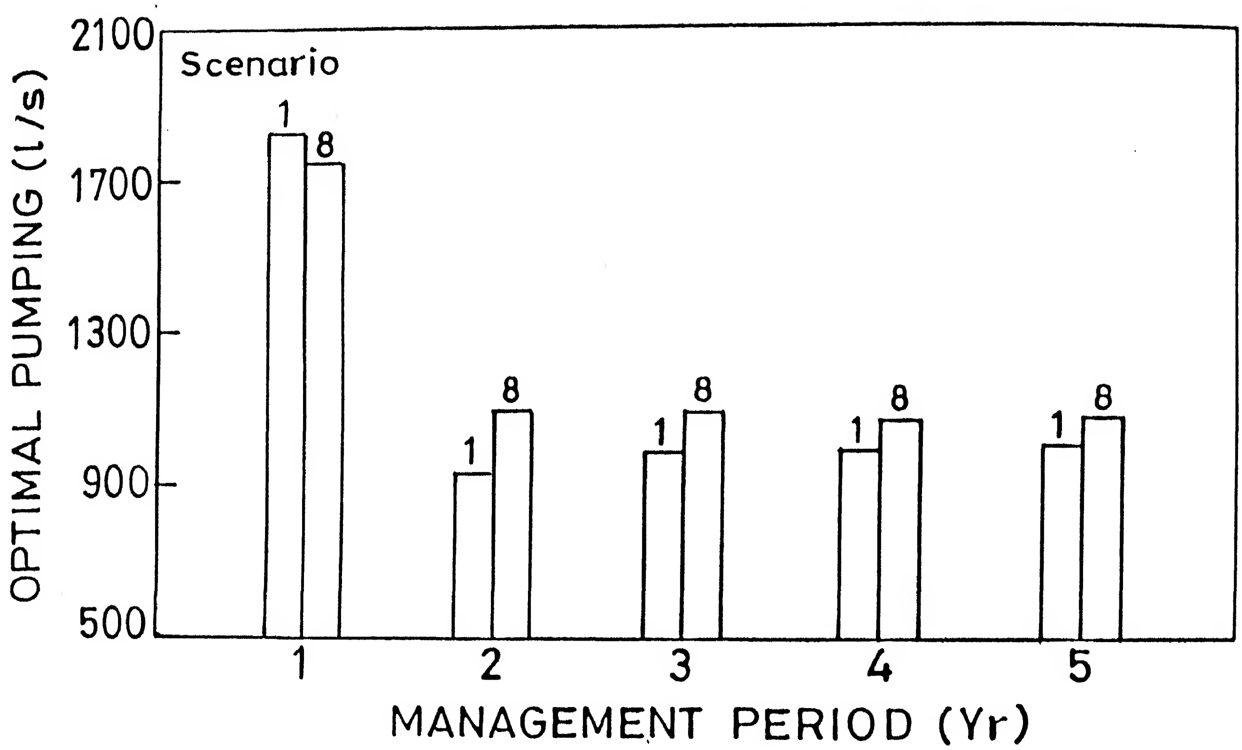


Fig. 6.1.16 Effect of leakage and recharge on transient optimal pumping.

solution is globally optimal. Hence, the pumping schedule reported here for different management scenarios may not be the optimal solution on global scale. It becomes evident from the fact that if the initial solution is changed then optimal solution also changes.

Table 6.1.7 gives the variation in the optimal values of objective and composite objective function with different initial guesses. The solution obtained with one set of initial solution may lead to a local optimum. A solution close to the global optimal can be established only by making a large number of runs with a large number of initial solution sets. The comparison of optimal solutions for different imposed physical and managerial constraints as mentioned earlier are useful in demonstrating the relative difference in the obtained solutions. The absolute magnitudes of these solutions are no doubt dependent on the fact whether the global optimal has been identified in each case or not. To see the nature of the composite objective function, its variation with decision variables at node (2,2) in first management period is shown in Fig. 6.1.17. It is clear from this figure that the composite objective function is most likely a nonconvex function and hence, a local optimal can not be guaranteed as a global one.

The simplest and most widely used approach to find the global optimum is the Multistart Strategy (MS). It involves multiple optimization runs, each initiated at a different starting point (initial solution). The level of confidence in getting global optimum can be enhanced by a large number of such optimization runs, because, only

Table 6.1.7 Effect of variation in initial solution on optimal value for scenario 1

Initial solution set	Order of violation of simulation constraints		Objective function value	
[$\underline{h}$, $\underline{P}$, $\underline{C}$]	Flow	Transport	F	ϕ
[m, l/s, mg/l]	(in S.I. unit)		(l/s)	(in S.I. unit)
[40, 50, 100]	10^{-9} - 10^{-14}	10^{-9}-10^{-13}	5736.70	-4.2060
[40, 500, 100]	10^{-10}-10^{-12}	10^{-9}-10^{-12}	9384.02	-7.6200
[40, 5000, 100]	10^{-10}-10^{-11}	10^{-9}-10^{-12}	9745.77	-9.4609

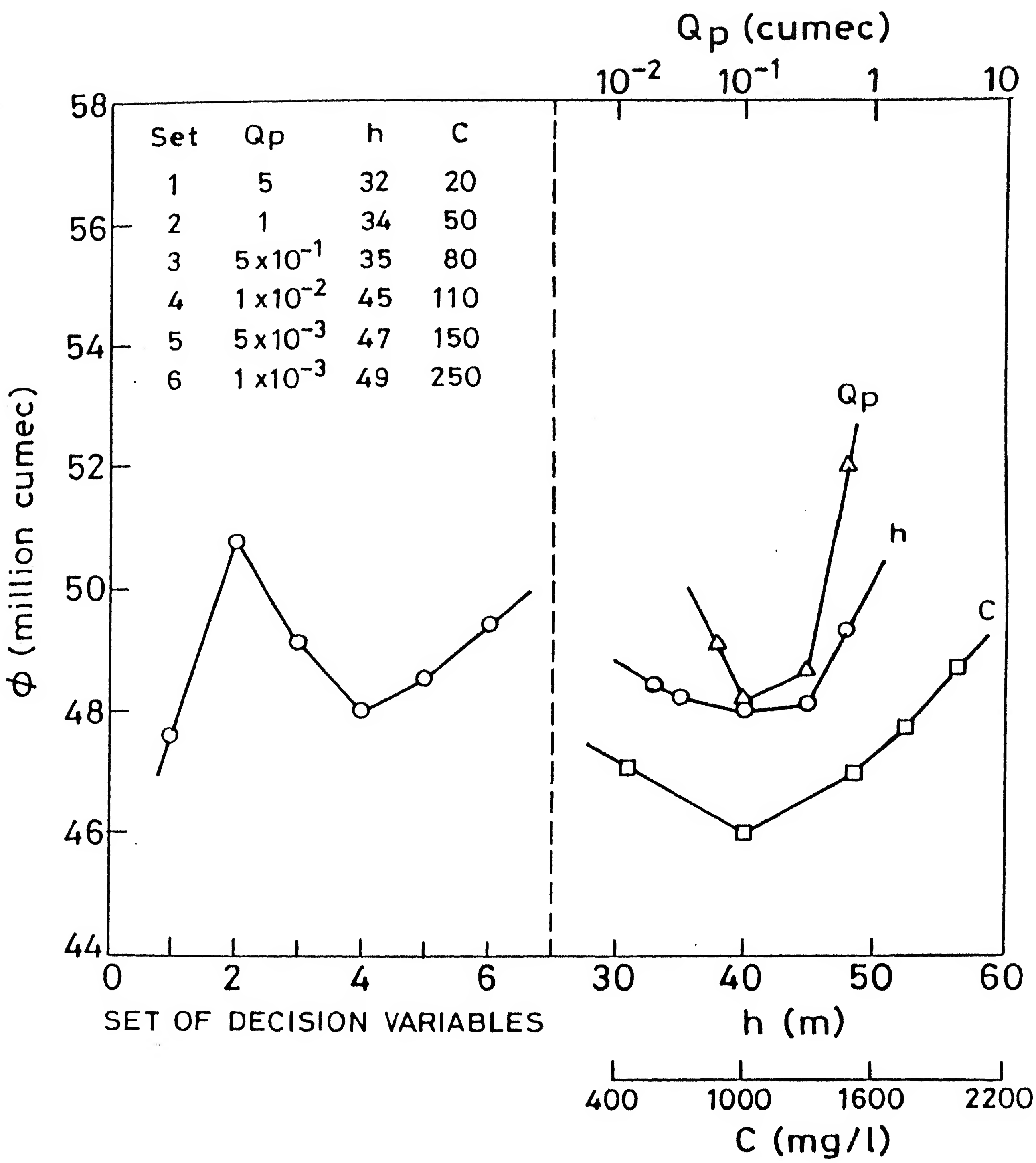


Fig.6.1.17 Variation of composite objective function with decision variables at node (2,2) in first management period.

then a large number of local optima are obtained for comparison.

6.1.8 Summary

The Hooke-Jeeves method in conjunction with exterior penalty function method can be successfully employed for a fairly large size of study area and also for large time horizons in the context of a transient groundwater management problems. The CPU time required to obtain the optimal solution for a management scenario depends upon the number of decision variables encountered in the planning and presence of physical and managerial constraints. The prescribed management strategies depend upon the boundary conditions, initial conditions, aquifer parameter estimates, presence of leaky layer and recharge load on the aquifer. In addition to these, quality of leakage from the overlying stratum, quality of recharge recharge, and managerial constraints influence the management policies more stringently. The global optimum solutions for different management scenarios can be guaranteed only when an exhaustive number of local optima are identified. This is an inherent problem of nonlinear optimization for nonconvex functions.

INTEGRATED MANAGEMENT FOR GROUNDWATER REMEDIATION

6.2 INTEGRATED MANAGEMENT FOR GROUNDWATER REMEDIATION

Contamination of groundwater is becoming an acute problem these days in all industrialized, urbanized and even rural areas due to various natural and man-made activities. In some regions, the quality of groundwater has deteriorated to such an extent that it is no longer fit for basic utilizations. In such areas, some remediation measures are needed to restore the aquifer, at least partially. This section is devoted to the enumeration of optimal management policies for the aquifer remediation. The goal is to decontaminate the aquifer by a planned withdrawal strategy.

The groundwater remediation problem is represented by Model II which is a minimization problem as discussed in Chapter 3. It aims at finding the time varying optimal policies to restore the aquifer under different physical and operational conditions. Parametric study is also carried out to assess the influence of the planning period. The effect of specified pumping locations on optimal policies and the global optimality of the solution results are also discussed.

6.2.1 Description of the study area

Fig. 6.2.1 shows the finite difference network for the study area of 900 ha (3 km x 3 km) with specified boundary condition. The boundaries towards North and South directions represent the constant head boundaries, and the remaining two sides of the area represent the impervious boundaries. The model is evaluated for a number of

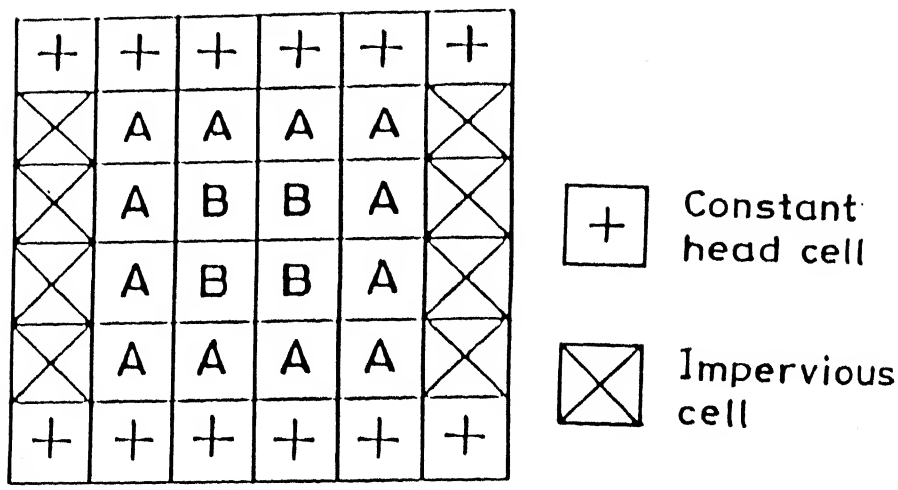


Fig. 6.2.1 Finite difference network .

different management scenarios. The characteristic of these scenarios are described in Table 6.2.1. The aquifer is assumed homogeneous and anisotropic for all management scenarios. The values of hydraulic conductivities K_{xx} and K_{yy} are assumed 5.0×10^{-4} m/s and 4.0×10^{-4} m/s respectively. The storage coefficient, effective porosity, thickness of leaky layer, saturated thickness of confined aquifer, hydraulic head in source bed and ground surface elevation are respectively 2.0×10^{-4}, 0.3, 2.0 m, 30.0 m, 55.0 m, and 62.0 m. These values do not change with respect to space and time.

Scenario 13 represents a case of confined aquifer with no leakage and recharge, whereas scenario 14 represents a case of leaky confined aquifer with recharge. The vertical hydraulic conductivity of overlying leaky layer in case of scenario 14 is assumed 1.0×10^{-8} m/s. The vertical point recharge due to waste injection or some other activities in all the internal cells (scenario 14) is 1.0 l/s throughout the management period. The solute considered here is chloride, a conservative pollutant. The concentrations of chloride entering the internal cells denoted by A and B (Figs. 6.2.1) are respectively 200 mg/l and 300 mg/l in recharge, and 50 mg/l and 100 mg/l in leakage (scenario 14). Scenario 15 represents a modified version of scenario 13, in which pumping takes place only from a limited number of specified wells. The longitudinal and transverse dispersivities are 30 m and 10 m respectively. Two time frames are considered for the analyses.

The hydraulic heads in constant head boundaries are specified

Table 6.2.1 Description of management scenarios (Remediation problem)

Management scenario	Leakage	Recharge	Remark
13	n	n	All cells are considered as decision variables for pumping
14	y	y	All cells are considered as decision variables for pumping
15	n	n	Limited cells are considered as decision variables for pumping

y exists; n does not exist

as 50.0 m at the top layers and 41.0 m at the bottom layers (Fig. 6.2.1). For the remaining cells, simple interpolation is used to obtain the hydraulic head distribution. This distribution is considered as the specified initial heads in the aquifer domain. Existing concentrations at all boundary cells are specified as zero. The initial concentration in the aquifer for the cells denoted by A and B (Fig. 6.2.1) are 100 mg/l and 350 mg/l respectively. All boundary cells are having zero concentration.

The inbuilt lower and upper bounds on hydraulic heads are respectively the top of the confining layer and the ground surface. The upper bounds on pumping variables are determined on the basis of capacity of maximum two pumps each of 80 H.P. with assumed efficiency of 65 percent. On the basis of this consideration the upper bound on pumping variables is found to be equal to 200 l/s. The inbuilt lower bounds are simply nonnegative. It is desired to restore the quality of groundwater upto a desired standard. To make the aquifer free from contamination, it is desired that the concentration of chloride should not be more than 250 mg/l throughout the aquifer by the end of the total planning period for remediation. This serves as the upper bound for concentration variables. The inbuilt lower bound on concentration variables are generally specified as zero to guarantee nonnegative values.

6.2.2 General discussion of results

The solutions of different management scenarios are obtained using Hooke-Jeeves method in conjunction with exterior penalty function method. The optimization parameters used for the computation are $r = 10^{-18}$, $\alpha_h = \alpha_q = \alpha_c = 2$ and $\beta_h = \beta_q = \beta_c = 1$. The search is started with initial guesses of 40 m for hydraulic head variables, 50 l/s for pumping variables and 100 mg/l for concentration variables. The initial step sizes are taken as 0.5 m for hydraulic head variables, 5.0 l/s for pumping variables and 10 mg/l for concentration variables. The values of termination parameters, ε_h, ε_q and ε_c are 0.001 m, 0.01 l/s and 0.01 mg/l respectively. The optimal solutions of different management scenarios are summarized in Table 6.2.2. The order of violation again represents a magnitude equal to the product of a fractional number (< 1) with the values reported in this table.

It is evident from Table 6.2.2 that the optimal solution obtained for various management scenarios fully satisfy simulation constraints as the order of violation of flow and transport equations for different cells in different times are negligible. The optimal pumping policies in first and second management periods (each of duration 180 days) that maintain the desired quality throughout the aquifer domain, at the end of 360 days are presented in Tables 6.2.3-6.2.5 for the scenarios 13-15 respectively. The solution results reported in these tables depict that the optimal policies depend upon the physical processes occurring within the

Table 6.2.2 Solution Results for management scenarios (Remediation problem)

Management scenario	optimal total pumping (l/s)
13	1033.81
14	1558.61
15	1058.48

Table 6.2.3 Optimal pumping policy for scenario 13

	Optimal pumping (l/s)			
i →	2	3	4	5
j ↓	1^{st} Management period			
2	0.00976	0.00976	0.00976	0.00976
3	0.00976	61.51400	79.50200	0.00976
4	0.00976	199.99000	199.99000	0.00976
5	0.00976	0.00976	0.00976	0.00976
	2^{nd} Management period			
2	0.00976	0.00000	0.00000	0.00000
3	0.00976	68.13500	93.45700	0.00976
4	0.00976	167.18000	163.84000	0.00976
5	0.00976	0.00976	0.00976	0.00976

Table 6.2.4 Optimal pumping policy for scenario 14

	Optimal pumping (l/s)			
i →	2	3	4	5
j ↓	1^{st} Management period			
2	45.25400	25.77100	34.57000	34.03300
3	3.42770	109.17000	129.83000	0.22461
4	0.00976	119.02000	126.53000	0.02930
5	30.72300	34.46300	24.80500	49.57000
	2^{nd} Management period			
2	50.95700	50.40000	69.54100	40.89800
3	44.77500	59.10200	56.87500	47.71500
4	0.00976	103.46000	114.61000	2.60740
5	50.36100	37.41200	25.40000	37.05100

Table 6.2.5 Optimal pumping policy for scenario 15

	Optimal pumping (l/s)			
i →	2	3	4	5
j ↓	1^{st} Management period			
2	0.00000	0.00000	0.00000	0.00000
3	0.00000	67.88100	71.37700	0.00000
4	0.00000	199.99000	199.99000	0.00000
5	0.00000	0.00000	0.00000	0.00000
	2^{nd} Management period			
2	0.00000	0.00000	0.00000	0.00000
3	0.00000	44.56100	74.69700	0.00000
4	0.00000	199.99000	199.99000	0.00000
5	0.00000	0.00000	0.00000	0.00000

aquifer system and operational conditions. Thus, to adopt an efficient strategy to remove the pollutants from the aquifer by using a planned withdrawal strategy, adequate and accurate modeling of the system is necessary in addition to the analyses of different alternatives available. Figs. 6.2.2-6.2.4 show the resulting spatial distribution of concentration for scenarios 13-15 respectively. These figures also show how the contaminated zone is reduced in areal extent in subsequent times due to pumping. The contaminated zone for different scenarios goes on reducing in size with time due to time varying optimal pumping at optimal locations.

In all the solution results reported here, Reynolds and Courant numbers are less than one, and hence obey the modeling requirements. The Peclet number is approximately 2.5 at initial condition, whereas at optimal condition, it varies between 4 and 10. Thus, convective dispersion dominates over molecular diffusion in all scenarios considered for the groundwater remediation problem.

Although the solutions have been obtained for a smaller sized area and for a less number of time steps, the model is equally applicable for larger sized area and for a large number of time steps. The basic idea behind taking smaller area and less number of time steps is to just reduce the CPU time required for one optimization run.

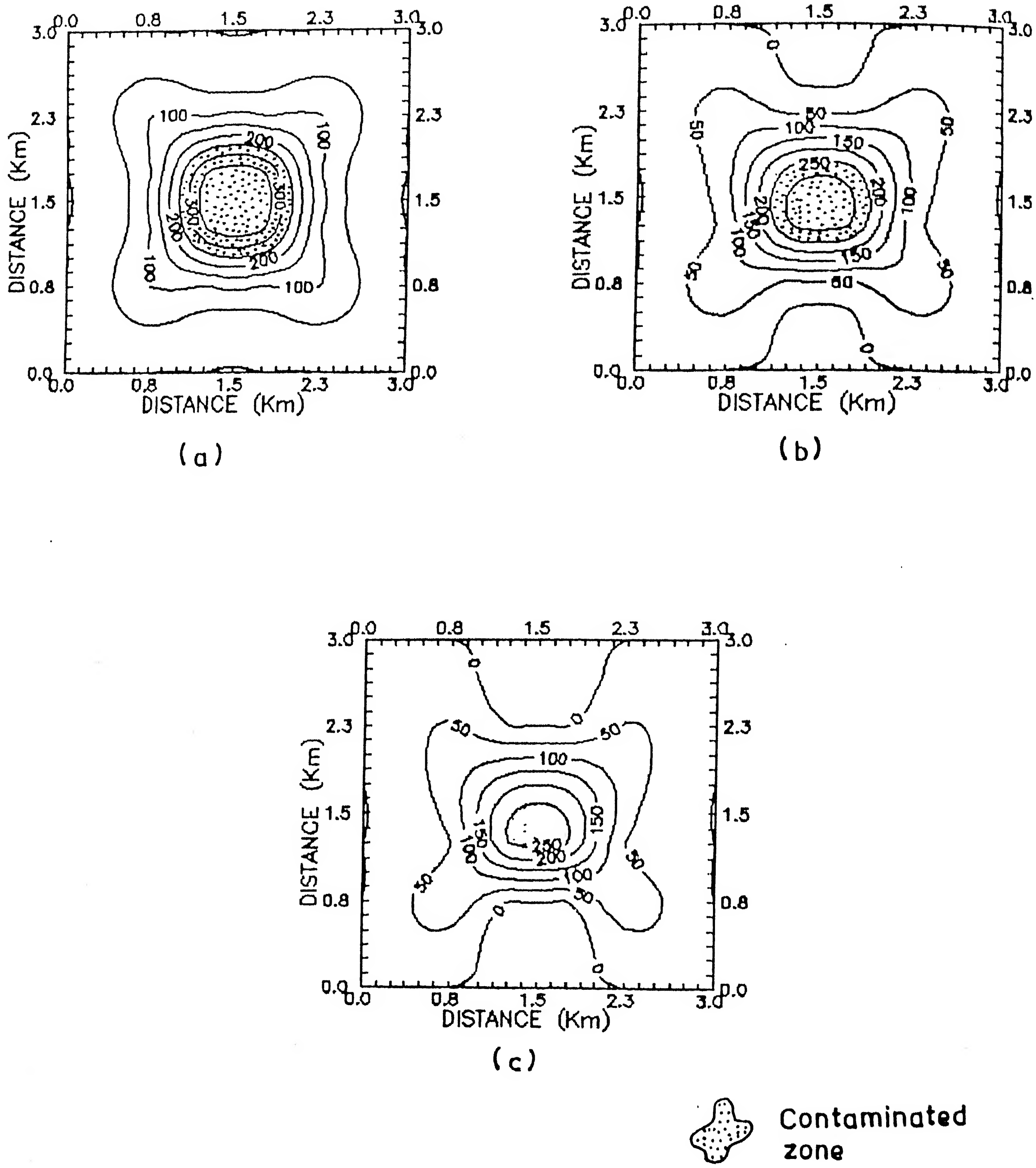


Fig. 6.2.2. Spatial distribution of concentration for scenario 13 at (a) t = 0 (b) t = 180 days (c) t = 360 days .

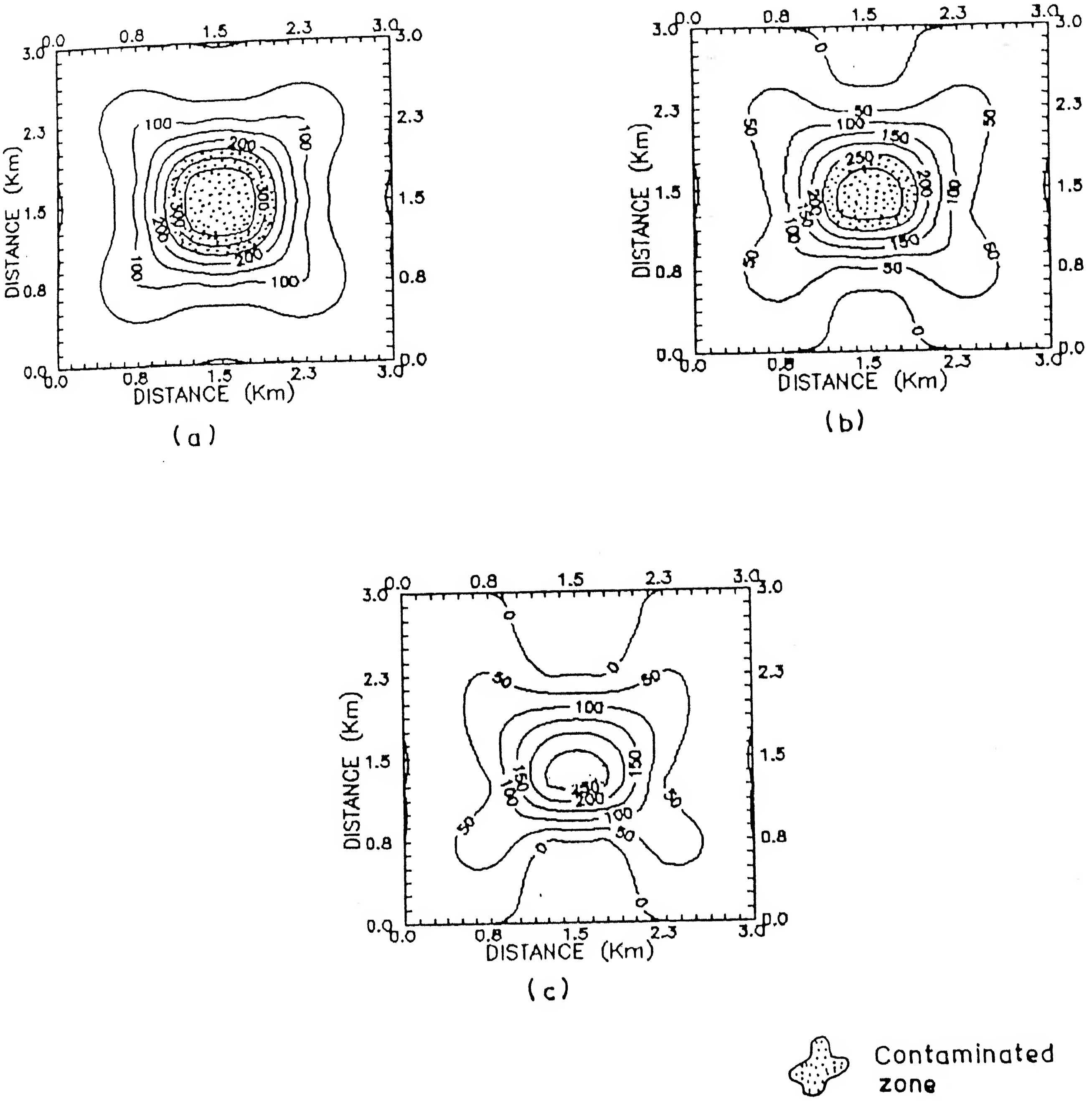


Fig. 6.2.3. Spatial distribution of concentration for scenario 14 at (a) t = 0 (b) t = 180 days (c) t = 360 days.

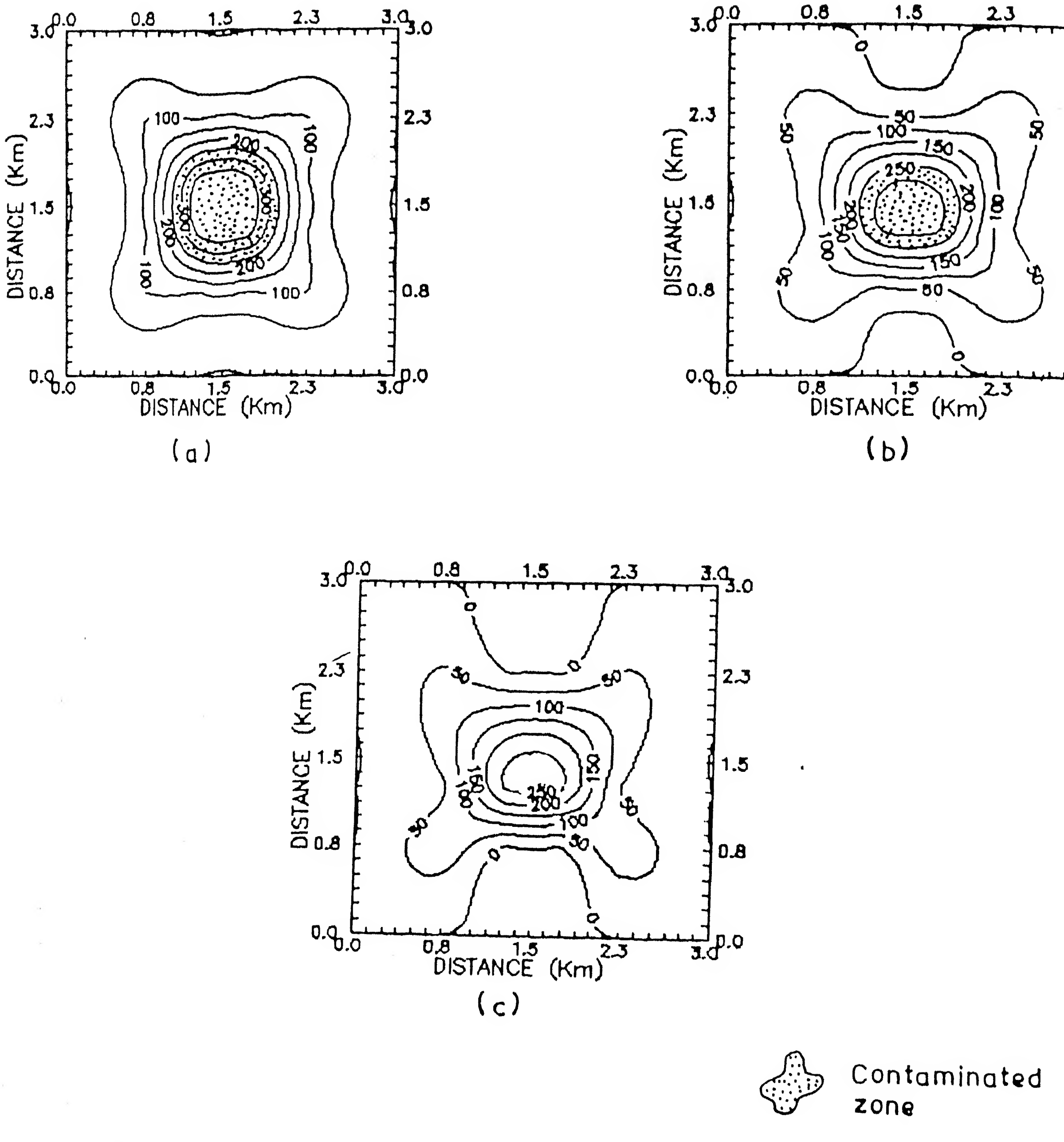


Fig. 6.2.4 Spatial distribution of concentration for scenario 15 at (a) t = 0 (b) t = 180 days (c) t = 360 days.

6.2.3 Sensitivity to planning period

The optimal total pumping from the aquifer required to maintain the desired quality throughout the aquifer domain decreases as the total planning period is increased (Table 6.2.6). The results reported in this table are obtained for scenario 13. Thus, to achieve the desired quality in shorter period, larger amount of pumping from the aquifer will be necessary. This will induce steeper hydraulic gradient to wash out the pollutant from the aquifer system. The required pumping reduces by 20.16% if the contamination is desired to be removed in 480 days instead of 360 days. However, if the aquifer is to be freed from contamination in only 300 days instead of 360 days, the required total pumping from the aquifer increases by 10.40%. The parametric variation of required optimal total pumping with planning period is shown in Fig. 6.2.5.

More pumping causes steeper hydraulic gradient. A very short planning period for cleaning up the aquifer may not be practicable, because, the heavy pumping requirement may have various adverse effects. Induced excessive hydraulic gradient may cause undesirable effects in the area such as subsidence, high infiltration, or, some other undesirable hydraulic connections with a different aquifer or a local water body. Therefore, a suitable planning period is chosen with due consideration of all such phenomena. The optimal pumping locations and the number of such locations for different planning periods in the area under consideration are also tabulated in Table 6.2.6. The total cost of pumping associated with each planning

Table 6.2.6 Variation of optimal solution with planning period

Planning period (days)	Optimal total pumping (l/s)
300	1141.28
360	1033.81
420	942.26
480	825.34

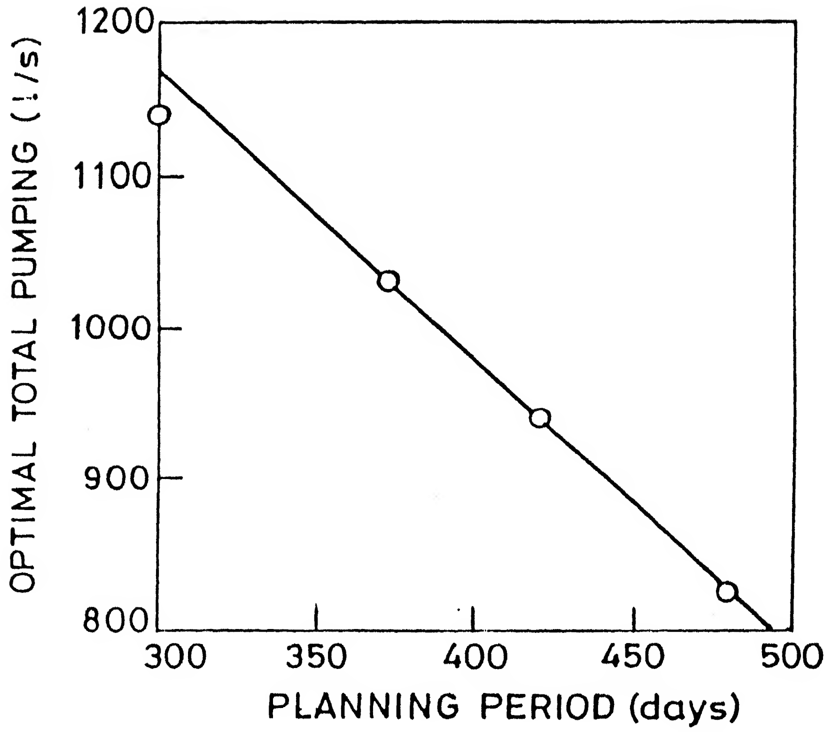


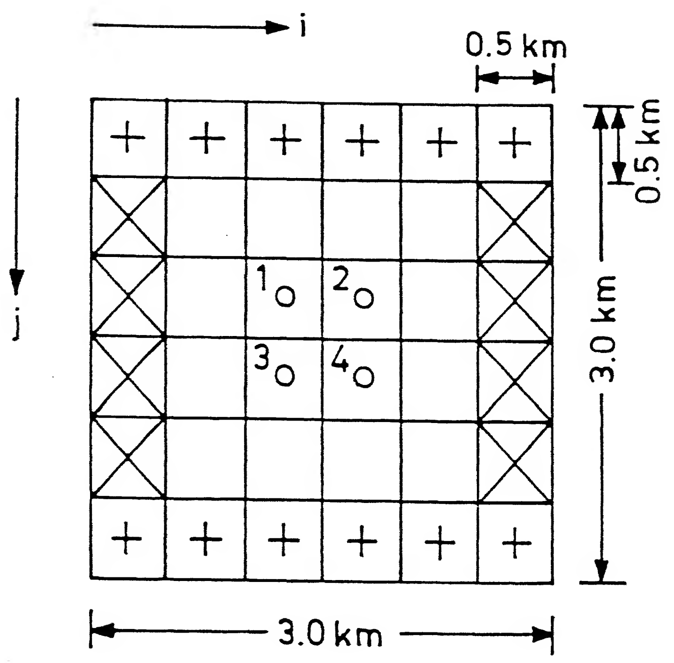
Fig. 6.2.5 Parametric variation of optimal total pumping with planning period.

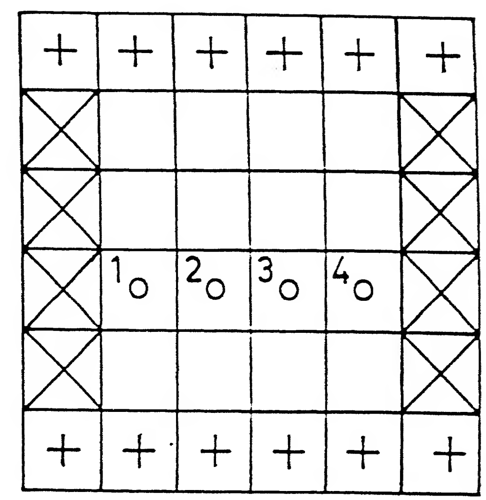
period can be assessed on the basis of all these three information provided in this table.

6.2.4 Specified potential pumping locations vs. optimally determined pumping locations

In many real life situations, pumping wells already exist in the area and it is required to decontaminate the aquifer by withdrawal from these potential pumping locations to avoid the additional cost of installing new wells. Such a situation is designated by scenario 15. The specified potential pumping locations in this scenario are shown in Fig. 6.2.6. The optimal pumping required from these specified pumping locations in first and second management periods is shown in Table 6.2.5. If the optimal pumping locations are also to be determined (scenario 13), the optimal pumping values at the potential locations specified in scenario 15 for both the scenarios 13 and 15 are shown in Table 6.2.7 for comparison. This comparison shows that pumping schedule from these specified locations will differ between the scenarios appreciably. However, if the specified potential pumping locations are identical to the optimally determined pumping locations, the difference in the pumping schedule will be marginal. It is evident from Table 6.2.8 that although total number of specified potential pumping locations are kept same, optimal pumping differs if its locations are varied (Fig. 6.2.7).

The optimal total pumping required to remediate the aquifer is





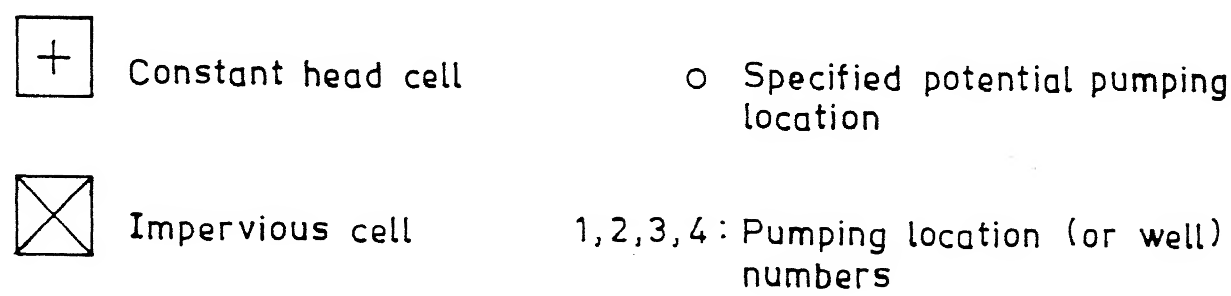


Fig. 6.2.6 Specified potential pumping locations for scenario 15.

Fig. 6.2.7 Specified potential pumping locations for a specific case of scenario 15.

Table 6.2.7 Comparative study of optimal pumping from specified potential pumping locations for scenarios 13 and 15

Well location (i, j)	Optimal pumping (l/s) 1st Management period		2nd Management period	
	scenario 13	scenario 15	scenario 13	scenario 15
(3, 3)	61.51400	67.88100	68.13500	44.56100
(4, 3)	79.50200	71.37700	93.45700	74.69700
(3, 4)	199.99000	199.99000	167.18000	199.99000
(4, 4)	199.99000	199.99000	163.84000	199.99000

Table 6.2.8 Effect of variability of specified potential pumping locations on optimal pumping

Well No.	Optimal pumping (l/s) 1st Management period		2nd Management period	
	scenario 15	special case of scenario 15	scenario 15	special case of scenario 15
1	67.88100	0.00000	44.56100	0.00000
2	71.37700	236.69000	74.69700	242.57000
3	199.99000	247.20000	199.99000	242.87000
4	199.99000	0.00000	199.99000	0.00000

lower when the well locations are determined optimally, the total cost of remediation will also include the cost of new well installations. Therefore, cost of installation and cost of pumping should be added together when new wells are needed. To make an effective cost analysis, the cost associated with the installation of new wells should also be taken into consideration. Such analysis should be augmented or these economic considerations should be explicitly included in the optimization model to devise an optimal policy that is cost effective at the same time.

6.2.5 Global optimality of management strategies

The solution results reported here can not be guaranteed to be the global optimal. It is because each reported solution has been obtained with only one set of initial guesses and for only one specified value of penalty parameter. The optimal solutions vary with different initial solution set as discussed in section 6.1. The problem of global optimality arises due to nonconvex nature of composite objective function. Fig. 6.2.8 shows the variation of composite objective function value with change in values of decision variables at node (2,2) in first management period. It is evident from this figure that this function is not unimodal and is convex in some region and nonconvex in some other region of the decision space. Nonconvexity problem will certainly become more acute when the variation of the composite objective function is observed with variations in all decision variables at a time. To overcome this

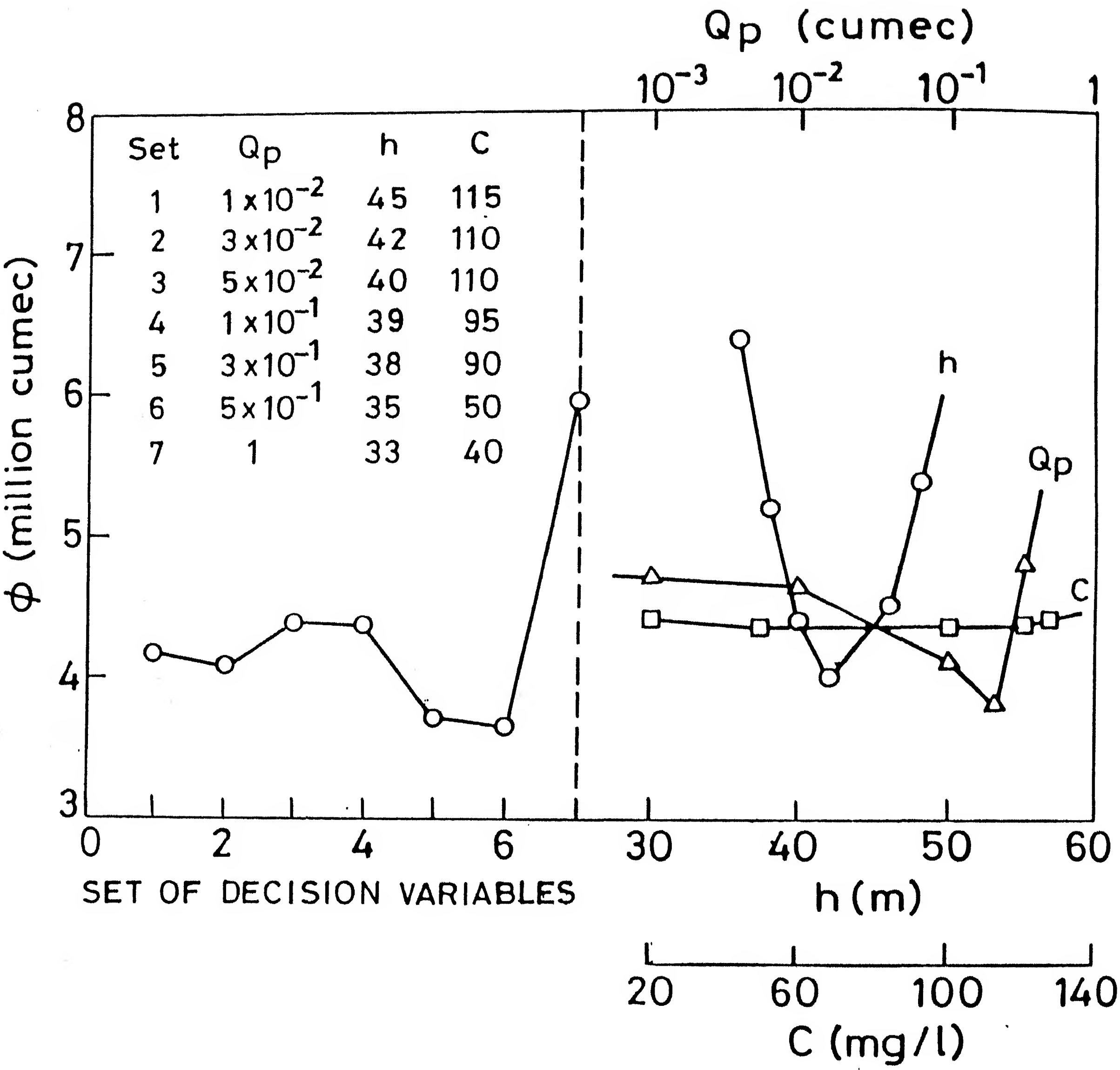


Fig. 6.2.8 Variation of composite objective function with decision variables at node (2,2) in first management period.

RADIONUCLIDE POLLUTANT MANAGEMENT

6.3 RADIONUCLIDE POLLUTANT MANAGEMENT

In section 6.1 of this Chapter, optimal solution of an integrated management model was presented, that deals with quality and quantity aspects together and maximizes groundwater withdrawal. The solutions satisfying the demand for various purposes in different aquifer environment and under different constraining situations were obtained and analyzed for a conservative pollutant, chloride. This section also deals with the maximization of groundwater withdrawal from the entire aquifer in a given planning horizon (Model I) with the modification that a decaying species, tritium, a radioactive pollutant is considered for the analysis. The solution of the model provides a time varying optimal management strategies for pumping locations together with the magnitudes of pumping rates from these locations. As a consequence, the resulting quality and hydraulic head distribution in space and time are also obtained. These solution results facilitate some other judgment on the quality and quantity aspects in qualitative or quantifiable units.

The solution results obtained for the performance evaluation of the model establish the suitability of the methodology. At the same time, these results are helpful in analyzing the groundwater management problems encountered in the areas where radioactive pollutant is of prime importance. However, actual policies to be implemented in a particular area will depend on the inputs of specific hydrologic conditions, and other imposed constraining

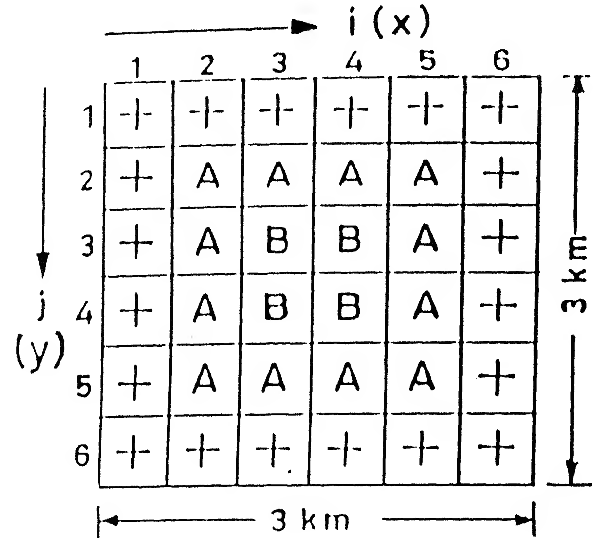
conditions applicable to that particular area of study.

The time varying spatially distributed optimal pumping policies are obtained for three types of boundary conditions. The optimal solutions are also obtained for different kinds of aquifer parameter estimates and imposed constraints to assess the significance of adequate modeling and the impact of restrictions on the optimal policies.

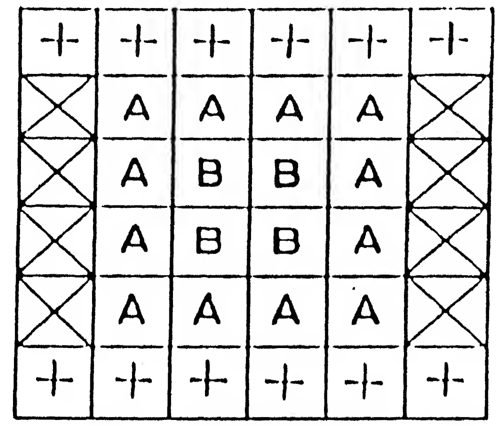
6.3.1 Description of the study area

The model is applied to two specified study areas. The finite difference network of the first study area (3 km x 3 km) with three different boundary conditions is shown in Figs. 6.3.1a-6.3.1c. The second study area represents a comparatively larger area (5 km x 5 km). The finite difference network for this study area with first kind of boundary condition (Dirichlet type) is shown in Fig. 6.3.1d. The model is evaluated for a number of different management scenarios accounting for the decay characteristic of tritium in advective-dispersive-diffusive-degradable solute transport equation. The characteristics of these scenarios are described in Table 6.3.1.

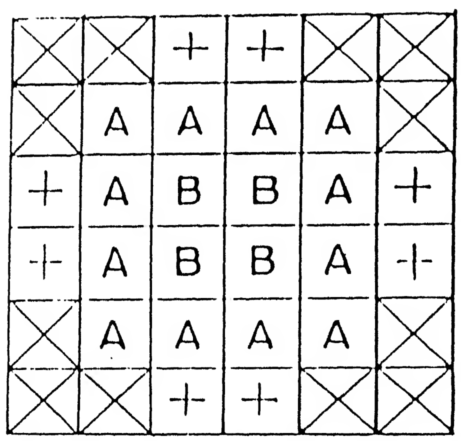
The aquifer is assumed homogeneous and anisotropic for the management scenarios 16-18 and 23-24. The management scenarios 19, 20 and 21 are based on the assumptions that the aquifer is respectively homogeneous and isotropic, heterogeneous and isotropic, and heterogeneous and anisotropic. For illustrative purpose, hydraulic conductivities for the scenarios 20 and 21 are estimated using exponential-



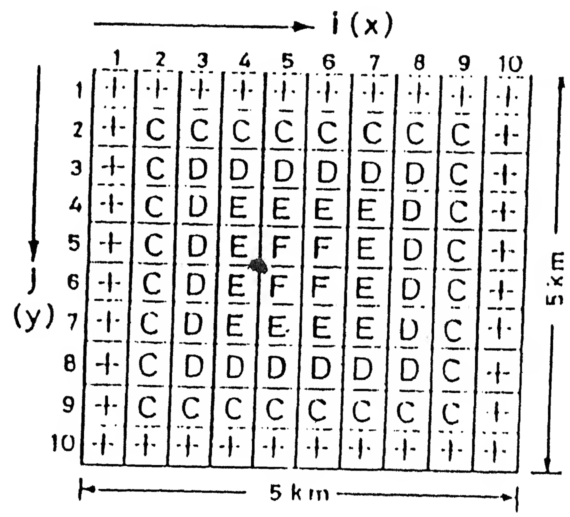
(a) Boundary condition type 1



(b) Boundary condition type



(c) Boundary condition type 3



(d) Larger study area with boundary condition type 1.

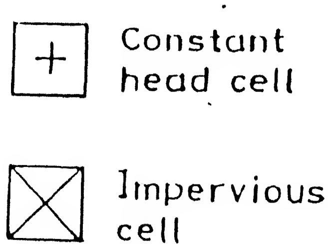


Fig. 6.3.1 Finite difference network.

Table 6.3.1 Description of management scenarios (Radioactive pollutant)

Management Scenario	Type of Boundary Condition	Hydraulic Conductivity (m/sec) K_{xx}	K_{yy}	Leakage	Recharge	Lower Bounds on h	P	C	Upper Bounds on h	P	C
16	1	5×10^{-4}	4×10^{-4}	y	y	i	i	i	i	n	n
17	2	5×10^{-4}	4×10^{-4}	y	y	i	i	i	i	n	n
18	3	5×10^{-4}	4×10^{-4}	y	y	i	i	i	i	n	n
19	1	4.5×10^{-4}	4.5×10^{-4}	y	y	i	i	i	i	n	n
20	1	HEI		y	y	i	i	i	i	n	n
21	1	HEA		y	y	i	i	i	i	n	n
22	1	Random HEA		y	y	i	i	i	i	n	n
23	1	5×10^{-4}	4×10^{-4}	y	y	y	y	i	i	y	y
24*	1	5×10^{-4}	4×10^{-4}	y	y	i	i	i	i	n	n

y exists
n does not exist
i inbuilt bound exists

HEI heterogeneous and isotropic
HEA heterogeneous and anisotropic
* For larger study area (10 km x 10 km)

ly varying deterministic expressions of the forms expressed by Equations 6.1 and 6.2. The values of K_o, a_{xx} (= a_{yx}) and a_{xy} (= a_{yy}) for scenario 20 are assumed 10^{-4} m/s, 0.395 km^{-1} and 0.295 km^{-1} respectively. The relative error in the mean value of computed hydraulic conductivities in this case is 0.43%. For the scenario 21, the values of K_o, a_{xx}, a_{xy}, a_{yx} and a_{yy} are assumed 10^{-4} m/s, 0.45 km^{-1}, 0.4 km^{-1}, 0.3 km^{-1} and 0.2 km^{-1} respectively. The relative errors in the mean values of computed K_{xx} and K_{yy} in this case are 0.85% and 0.25% respectively. Heterogeneous and anisotropic characteristic of the aquifer is also modeled using randomly generated spatial values of hydraulic conductivity (scenario 22). The hydraulic conductivity is assumed random in space following a Gaussian distribution with standard deviation of 20% of the mean. This mean value is assumed 5 x 10^{-4} m/s for K_{xx} and 4 x 10^{-4} m/s for K_{yy}. The relative errors in the mean values of computed hydraulic conductivities are 0.85% for K_{xx} and 1.35% for K_{yy}.

The storage coefficient, effective porosity, thickness of leaky layer, saturated thickness of confined aquifer, hydraulic head in source bed and ground surface elevation are respectively 2.0 x 10^{-4}, 0.3, 2.0 m, 30.0 m, 55.0 m, and 62.0 m. These values do not change in space and time. The vertical hydraulic conductivity of overlying leaky layer is 1.0 x 10^{-10} m/s in all the management scenarios where leakage exists. The vertical point recharge due to waste injection or some other activities in all the cells except boundary cells, when applicable is 1.0 l/s throughout the management period. The

recharge at all boundary cells is assumed zero. The radioactive pollutant considered here is tritium. Its concentration entering the internal cells denoted by A and B (Figs. 6.3.1a-6.3.1c) are respectively 10 μc/l and 5 μc/l in recharge, and 2 μc/l and 4 μc/l in leakage. The tritium concentration entering the internal cells denoted by C, D, E and F (Fig. 6.3.1d) are respectively 10 μc/l, 5 μc/l, 1.5 μc/l and zero in recharge, and 2 μc/l, 4 μc/l, 1 μc/l and zero in leakage. The longitudinal and transverse dispersivities are 30 m and 10 m respectively. Five time frames are considered for the scenarios 16-23, whereas for the scenario 24, the number of time frames considered are ten in a time horizon of five years.

The hydraulic heads at the outermost cells towards north and south are specified as 50.0 m and 41.0 m respectively (Figs. 6.3.1a-6.3.1d). For the remaining cells, simple interpolation is used to obtain the head distribution. The resulting hydraulic head distribution is considered as the specified initial heads. Existing concentrations at all boundary cells are specified as 1 μc/l for the first study area and zero for the second study area. The initial concentrations in the aquifer for the cells denoted by A, B, C, D, E and F (Fig. 6.3.1) are 10 μc/l, 2 μc/l, 10 μc/l, 2 μc/l, 1 μc/l and zero respectively.

The inbuilt lower and upper bounds on hydraulic head variables are respectively the top of the confining layer and the ground surface. However, these inbuilt bounds can be made redundant by imposing more constraining managerial lower and upper bounds. The

lower and upper bounds on pumping for scenario 23 are determined on the basis of irrigation demand and capacity of available pumping equipments respectively as discussed in Chapter 3. For example, assuming average climatic conditions of North India and 30% of each grid area under crop, the lower bound on pumping is estimated by accounting for both planting seasons in North India (Kharif and Rabi). The upper bound on pumping is determined on the basis of capacity of two pumps, each of 80 H.P. having 65% efficiency. These bounds for each cell are respectively 15 l/s and 200 l/s throughout the planning period. In case of inbuilt bounds where these straining bounds do not exist are simply nonnegative for lower bounds and none for upper bounds. For the concentration variables, the lower bounds are generally specified as zero to have nonnegative values, while upper bounds imposed are 2.0 μc/l where applicable. There is no inbuilt upper bound on concentration.

6.3.2 General discussion of results

To obtain the optimal solutions for various management scenarios, the optimization runs are started with initial values of 40.0 m, 50 l/s and 1.0 μc/l for hydraulic head, pumping and concentration variables respectively. The starting and final step sizes are assumed respectively 0.5 m and 0.001 m for hydraulic head variables, 5 l/s and 0.01 l/s for pumping variables, and 1.0 μc/l and 0.001 μc/l for concentration variables. The optimal solutions of various management scenarios for $r = 10^{-18}$, $\alpha_h = \alpha_q = \alpha_c = 2$ and β_h

$= \beta_q = \beta_c = 1$ are summarized in Table 6.3.2. This table gives the information about required CPU time, order of violation of flow and transport equations, optimal total pumping, optimal value of composite objective function, and number of function evaluations to obtain optimal values for different management scenarios. The order of violation represents a magnitude equal to the product of a fractional number (<1) with the values reported in Table 6.3.2. Table 6.3.3 shows the yearly optimal pumping policies for the entire aquifer for different management scenarios.

If the model is constrained more severely (scenario 23), the optimal total pumping reduces accordingly. The obtained solution may be very far from the solution obtained in more relaxed condition. The management scenario 24 demonstrates that the developed methodology can be applied to a larger sized study area for a longer time frame.

These results demonstrate the applicability, robustness and versatility of Hooke-Jeeves method in conjunction with exterior penalty function method to solve groundwater management problems dealing with quality and quantity aspects together, in different natural and operational situations. It is observed that this method is suitable for embedding technique which involves large number of variables and constraints to simulate the system. This investigation shows that even a larger sized study area for a large time span can be solved. The drawback is that it consumes a large CPU time in identifying even a single optimum solution of a dimensionally large

Table 6.3.2 Solution Results for Management Scenarios (Radioactive pollutant)

Management Scenario	No. of Decision Variables	No. of Simulation Constraints	CPU Time (Min.)	No. of Function Evaluations	Order of Violation of Constraints Flow (Transport) (in S.I. unit)	Optimal Total Pumping for 5-Yr. Planning Period (l/s)	Optimal Value of Composite Objective Function (in S.I. unit)
16	240	160	12.90	36546	10^{-10}–10^{-12} (10^{-9} –10^{-11})	4886.94	-3.9017
17	240	160	15.57	45204	10^{-10}–10^{-12} (10^{-9} –10^{-12})	2492.83	4.2278
18	240	160	20.41	57229	10^{-10}–10^{-12} (10^{-9} –10^{-15})	2943.19	5.8376
19	240	160	4.90	13939	10^{-10}–10^{-12} (10^{-9} –10^{-12})	5191.06	-2.7888
20	240	160	4.72	13548	10^{-10}–10^{-11} (10^{-9} –10^{-11})	4887.91	-2.5867
21	240	160	4.90	13939	10^{-10}–10^{-13} (10^{-9} –10^{-11})	4632.89	2.4815
22	240	160	4.54	12977	10^{-10}–10^{-11} (10^{-9} –10^{-11})	5017.18	-1.5790
23	240	160	6.21	17787	10^{-10}–10^{-14} (10^{-8} –10^{-13})	4627.17	629.5016
24	1920	1280	320.43	134425	10^{-9} –10^{-12} (10^{-8} –10^{-13})	19733.04	410.2869

Table 6.3.3 Yearly optimal pumping policies for management scenarios (Radioactive pollutant)

Management Scenario	Optimal pumping (l/s) in Management period (year)				
	1	2	3	4	5
16	977.49	977.36	977.36	977.36	977.36
17	498.69	498.53	498.53	498.53	498.50
18	587.99	588.84	588.79	588.79	588.79
19	1038.29	1038.19	1038.19	1038.19	1038.19
20	973.65	973.56	973.56	973.56	973.56
21	926.64	926.56	926.56	926.56	926.56
22	1003.54	1003.41	1003.41	1003.41	1003.41
23	847.62	847.42	977.40	977.36	977.36
24	3947.45	3946.30	3946.42	3946.42	3946.42

problem. The CPU time requirements presented in Table 6.3.2 show that as the number of decision variables are increased 8 times (scenario 16 and scenario 24), the CPU time required to obtain the optimal solution for a particular value of r increases approximately 25 times. It is evident from the Table 6.3.3 that optimal pumping policy for a particular scenario is almost constant throughout the management period.

However, if the CPU time required to obtain optimal solutions for different scenarios are compared with those required for the scenarios dealing with conservative pollutant only (Tables 6.1.2 and 6.3.2), it is observed that CPU time requirement in the former case is comparatively less. This is because of lesser magnitudes of radionuclide concentrations in the aquifer, and possibly due to a better guess of the initial solution vector. In this case a smaller length of travel in optimization search is required. This consequence is also highlighted if the magnitudes of the composite objective function at the beginning of search is compared for both the cases. The order of magnitude of the composite objective function at the beginning of search for the scenarios (applicable for the first study area) dealing with conservative pollutant is 10^8, whereas for the scenarios dealing with radioactive pollutant, it is 10^7. The problems associated with scaling and sparse constraint matrices generally do not affect the solutions adversely in this methodology. The effects of these problems are made insignificant by the modifications implemented in HJ algorithm as

discussed in Chapter 4. However, the solutions appear to be affected by the curse of local optimality because of nonconvex nature of the functions which is explained in section 6.3.5.

6.3.3 Effects of boundary conditions

Fig. 6.3.2 shows that optimal total pumping from the aquifer and thus, transient pumping policies will be different for different types of boundary conditions. Therefore, the management policies to be adopted for optimal pumping are dependent on the boundary conditions which exist in the aquifer domain under consideration. Presence of more constant head cells enable larger withdrawal from the aquifer due to increased potential recharge.

The optimal pumping policies in fifth management period for different specified boundary conditions represented by scenarios 16, 17 and 18 are given in Tables 6.3.4, 6.3.5 and 6.3.6 respectively. The resulting distributions of tritium concentration in the aquifer in fifth management period for these scenarios are shown respectively in Figs. 6.3.3a, 6.3.3b and 6.3.3c. As per the solutions, the water rushes towards the central area of the aquifer and thus pollutant tends to accumulate near this zone. However, pollutant's strength is diminished throughout the area because of pumping and recharge of fresh water from the boundary cells. The velocity field in fifth management period is shown in Fig. 6.3.4 for (a) scenario 16, (b) scenario 17, and (c) scenario 18. The hydraulic head distribution at the end of planning period is shown in Fig.

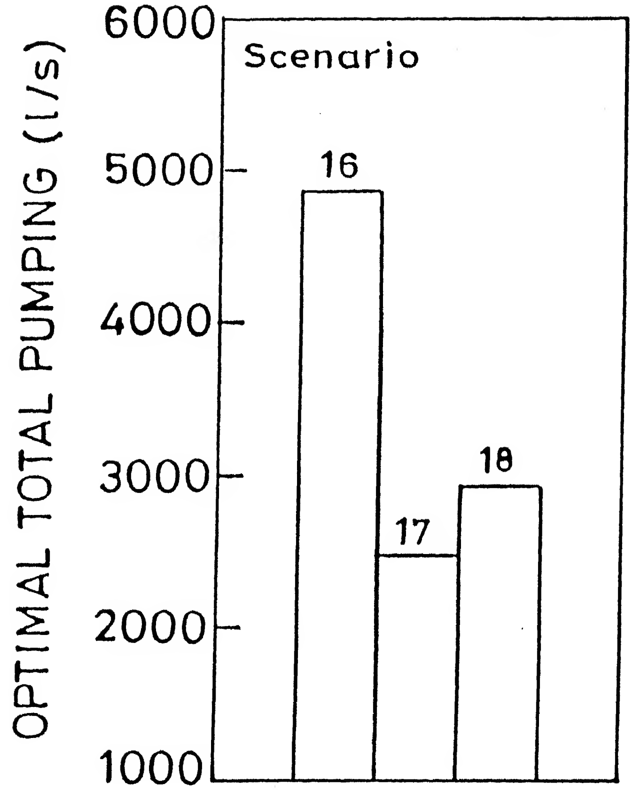


Fig. 6.3.2 Effect of specified boundary conditions on optimal total pumping.

Table 6.3.4 Optimal pumping policy in fifth management period for scenario 16

	Optimal pumping (l/s)			
i →	2	3	4	5
j ↓				
2	96.69	97.87	94.47	90.00
3	97.90	53.98	60.83	88.90
4	30.76	34.95	30.08	80.64
5	28.07	43.14	22.51	26.56

Table 6.3.5 Optimal pumping policy in fifth management period for scenario 17

	Optimal pumping (l/s)			
i →	2	3	4	5
j ↓				
2	62.75	62.75	65.17	76.47
3	21.68	20.46	18.25	18.53
4	19.02	19.21	19.21	18.46
5	19.14	19.14	19.14	19.14

Table 6.3.6 Optimal pumping policy in fifth management period for scenario 18

	Optimal pumping (l/s)			
i →	2	3	4	5
j ↓				
2	36.67	63.80	66.50	34.18
3	54.25	41.50	26.70	50.74
4	29.03	26.47	26.52	26.48
5	26.46	26.48	26.51	26.48

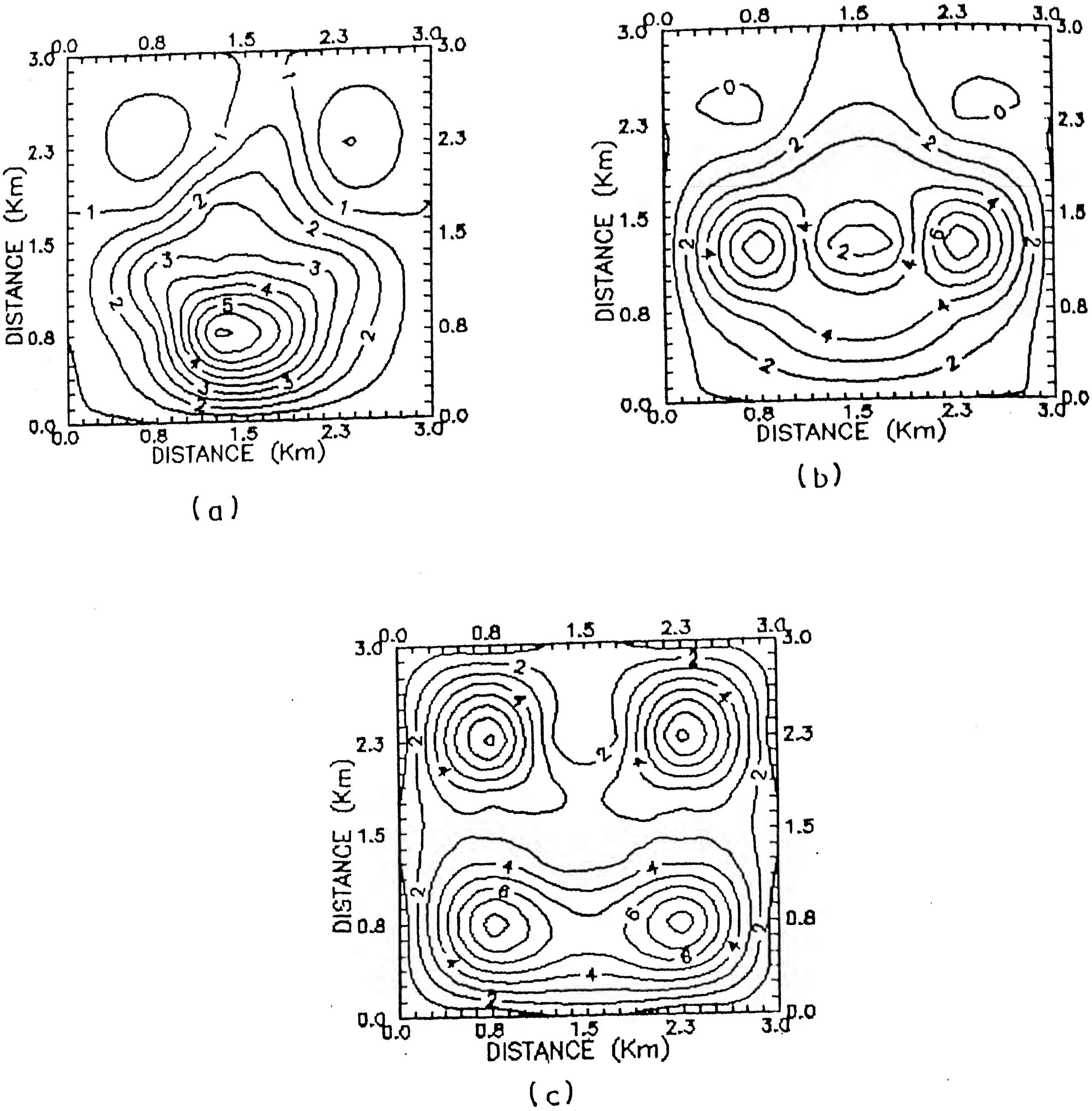


Fig. 6.3.3. Optimal spatial distribution of concentration in fifth year for (a) scenario 16 (b) scenario 17 (c) scenario 18.

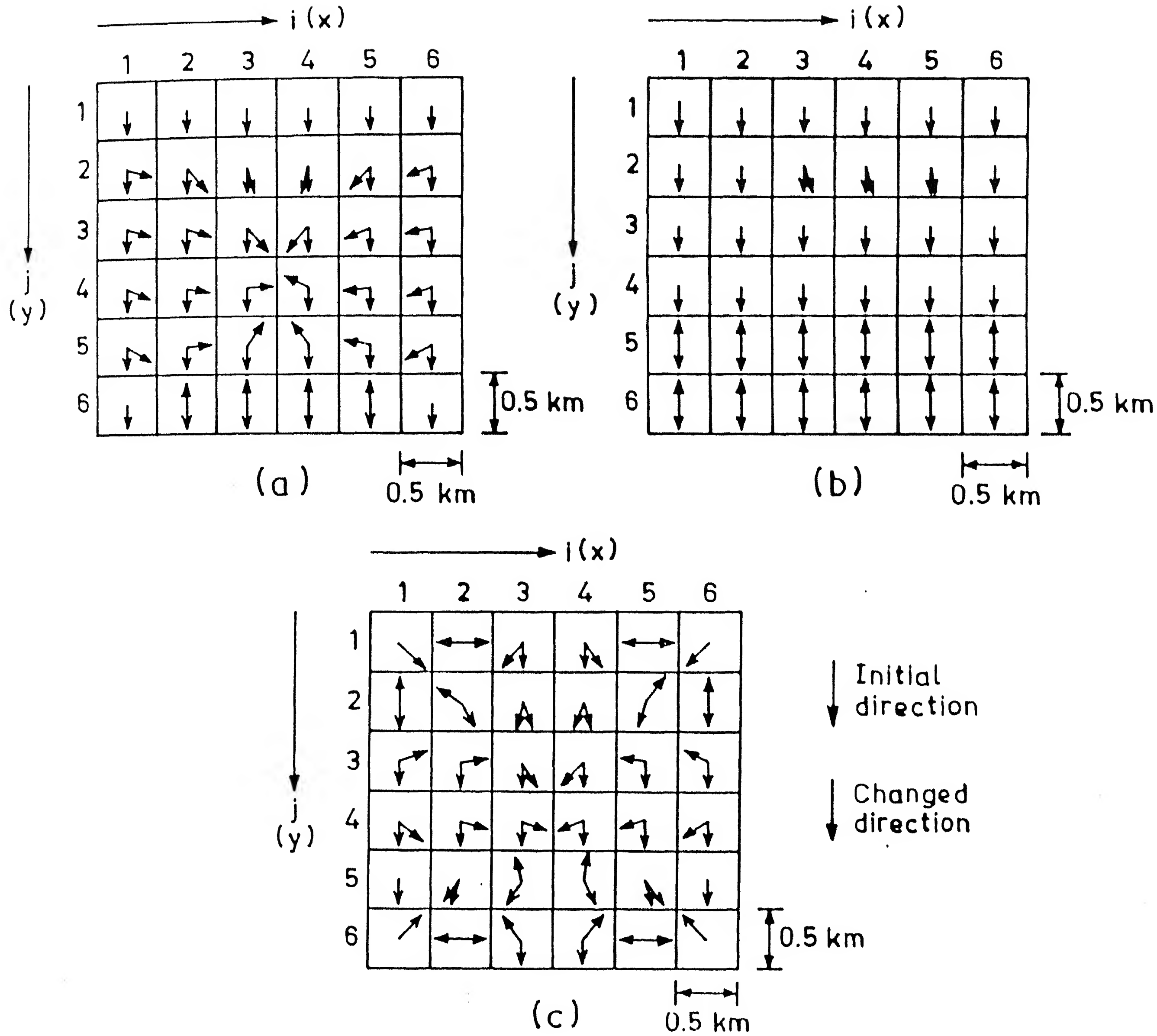


Fig. 6.3.4 Velocity field in fifth management period for
(a) Scenario 16 (b) Scenario 17 (c) Scenario 18.

6.3.5 for (a) scenario 16, (b) scenario 17, and (c) scenario 18.

6.3.4 Effect of aquifer parameter estimates

As discussed in case of conservative pollutant (section 6.1.5), the optimal management policies in case of radioactive pollutant also depend upon the nature of the aquifer medium. The heterogeneity and anisotropy of the aquifer system affect the optimal strategies. To obtain the true optimal strategies, it is required to estimate the aquifer parameters more adequately. Fig. 6.3.6 shows the effect of heterogeneity on optimal total pumping from isotropic and anisotropic aquifers. The effect of anisotropy on optimal total pumping from homogeneous and heterogeneous aquifers is shown in Fig. 6.3.7. These illustrations demonstrate the significance of accurate parameter estimation. The difference in the optimal solutions due to different methods adopted for the estimation of aquifer parameters will be more pronounced in real life situations.

Fig. 6.3.8 compares the optimal solutions obtained using deterministic and random modeling of heterogeneous and anisotropic hydraulic conductivity, with those obtained for simplified assumptions of homogeneity and isotropy. The randomized distribution of hydraulic conductivity is assumed to follow a Gaussian distribution with a standard deviation of 20% of the mean. The results shown in Figs. 6.3.6-6.3.8 emphasize the effects of modeling the hydraulic conductivity of the system adequately. Otherwise, the optimal management decision may vary appreciably reflecting

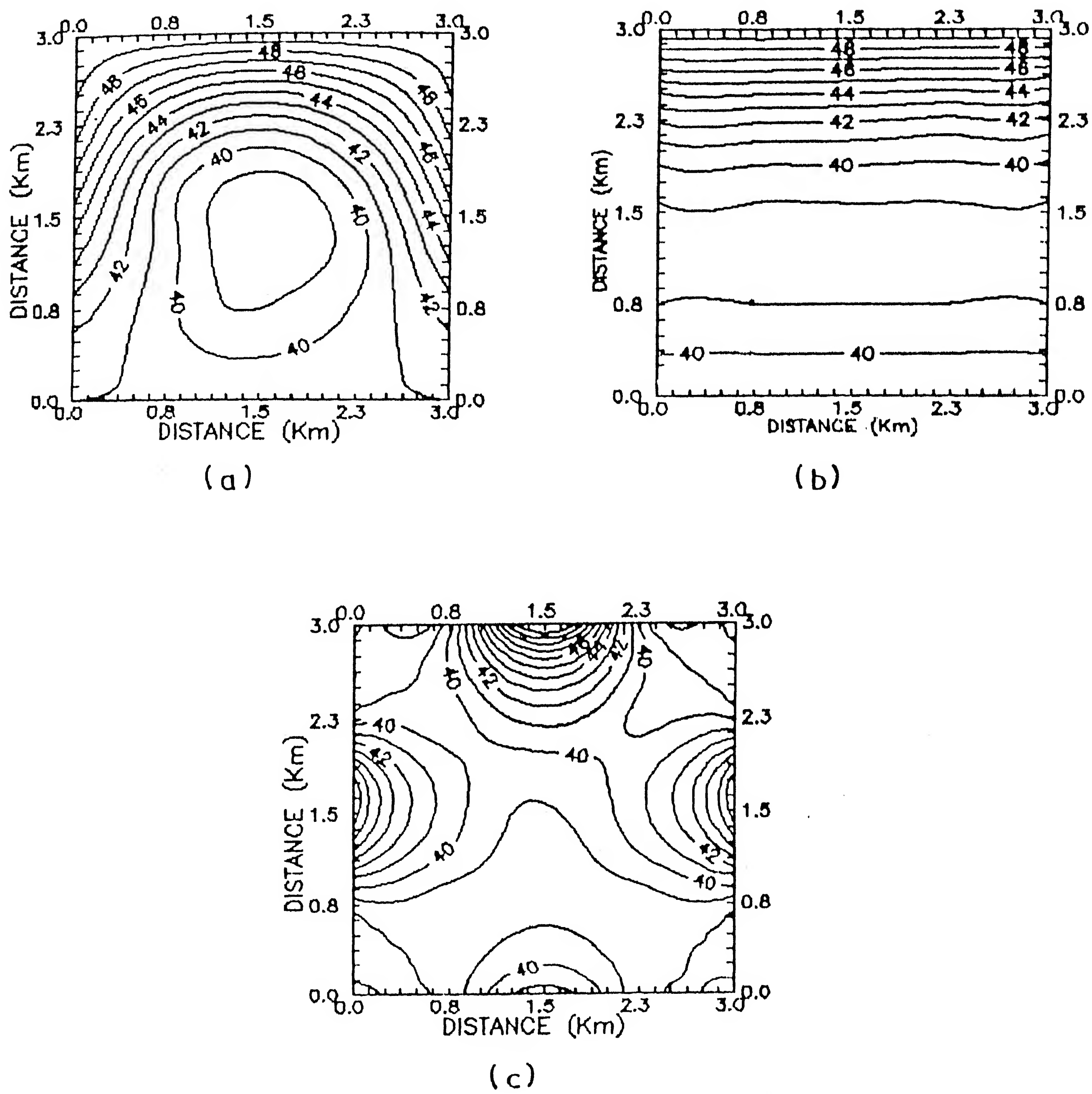


Fig. 6.3.5 Optimal spatial distribution of hydraulic head at the end of planning period for (a) scenario 16 (b) scenario 17 (c) scenario 18.

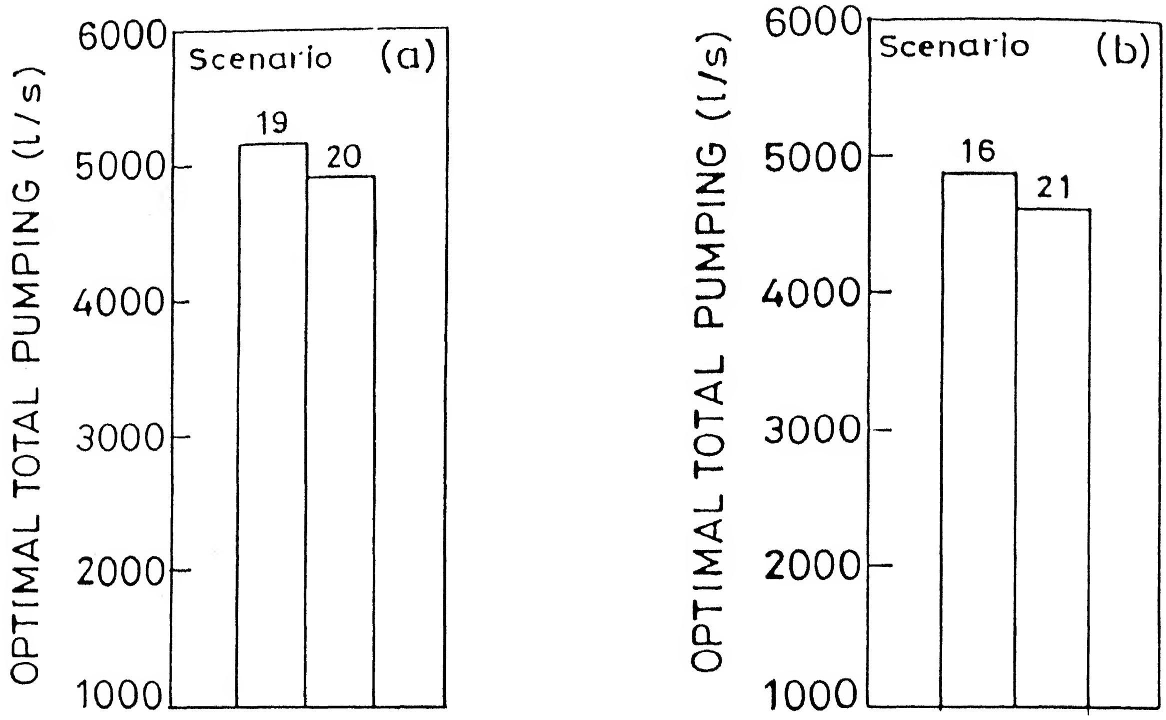


Fig. 6.3.6 Effect of heterogeneity on optimal total pumping from (a) isotropic aquifer (b) anisotropic aquifer.

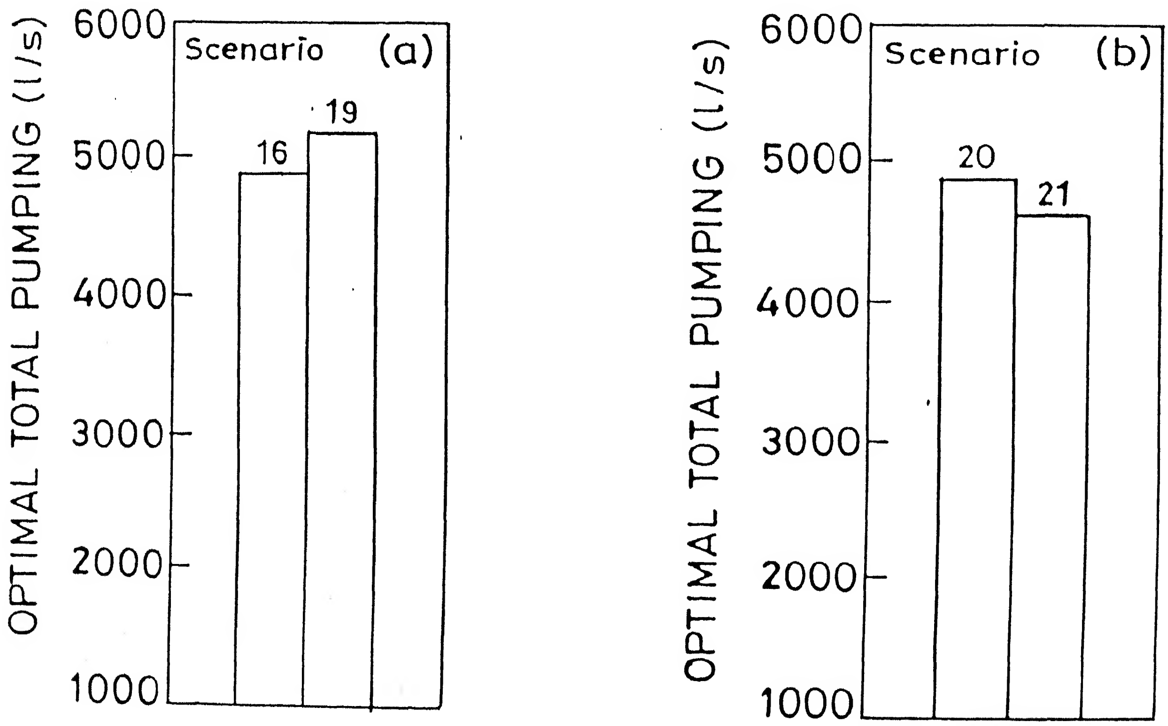


Fig. 6.3.7 Effect of anisotropy on optimal total pumping from (a) homogeneous aquifer (b) heterogeneous aquifer.

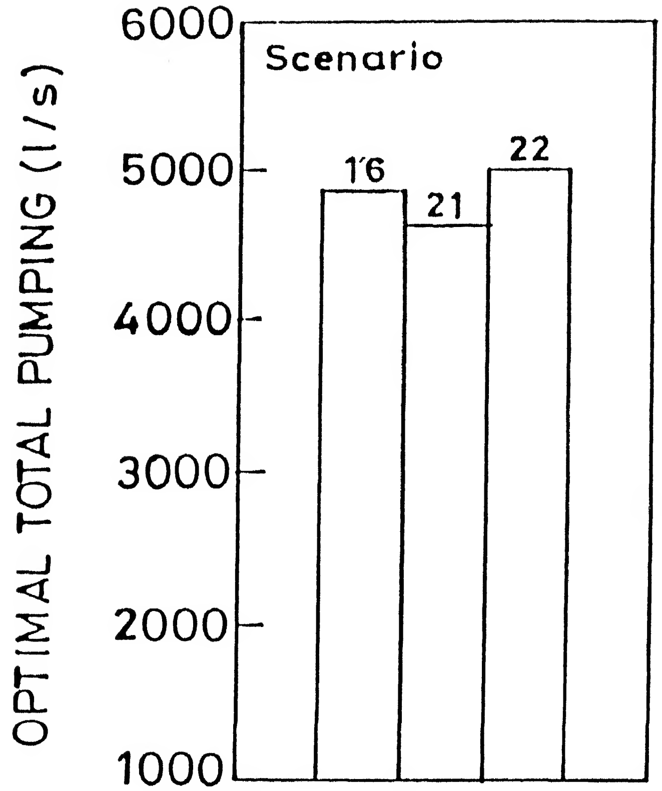


Fig. 6.3.8 Effect of deterministic and randomized modelling of hydraulic conductivity on optimal total pumping.

inadequate representation of the medium. The variations in the optimal pumping policies will be more pronounced if the spatial variations of other aquifer parameters such as dispersivity are also considered.

6.3.5 Global optimality of management strategies

The optimal results reported here are based on only one value of penalty parameter. At the optimal condition, the violation of constraints becomes negligible. The superior optimal solution may be achieved by performing more optimization runs with different values of penalty parameter as discussed in Chapter 5. However, the results reported here correspond to a penalty parameter value at which the optimal solution converges. The solutions reported in this section can be reasonably assumed to be global only when large number of optimization runs are performed for each scenario to be sure that all possible identified local optima are inferior. However, the subjective assessment of the sensitiveness of various parameters and impact of various physical and managerial situations remain valid, even without a guarantee of global optimum.

Table 6.3.7 gives the variation in the optimal values of objective and composite objective functions with different initial guesses for decision variables. It signifies that more number of optimization runs are needed to establish a global solution. However, it may be possible that a large number of optimization runs may not result in appreciable difference among obtained solutions.

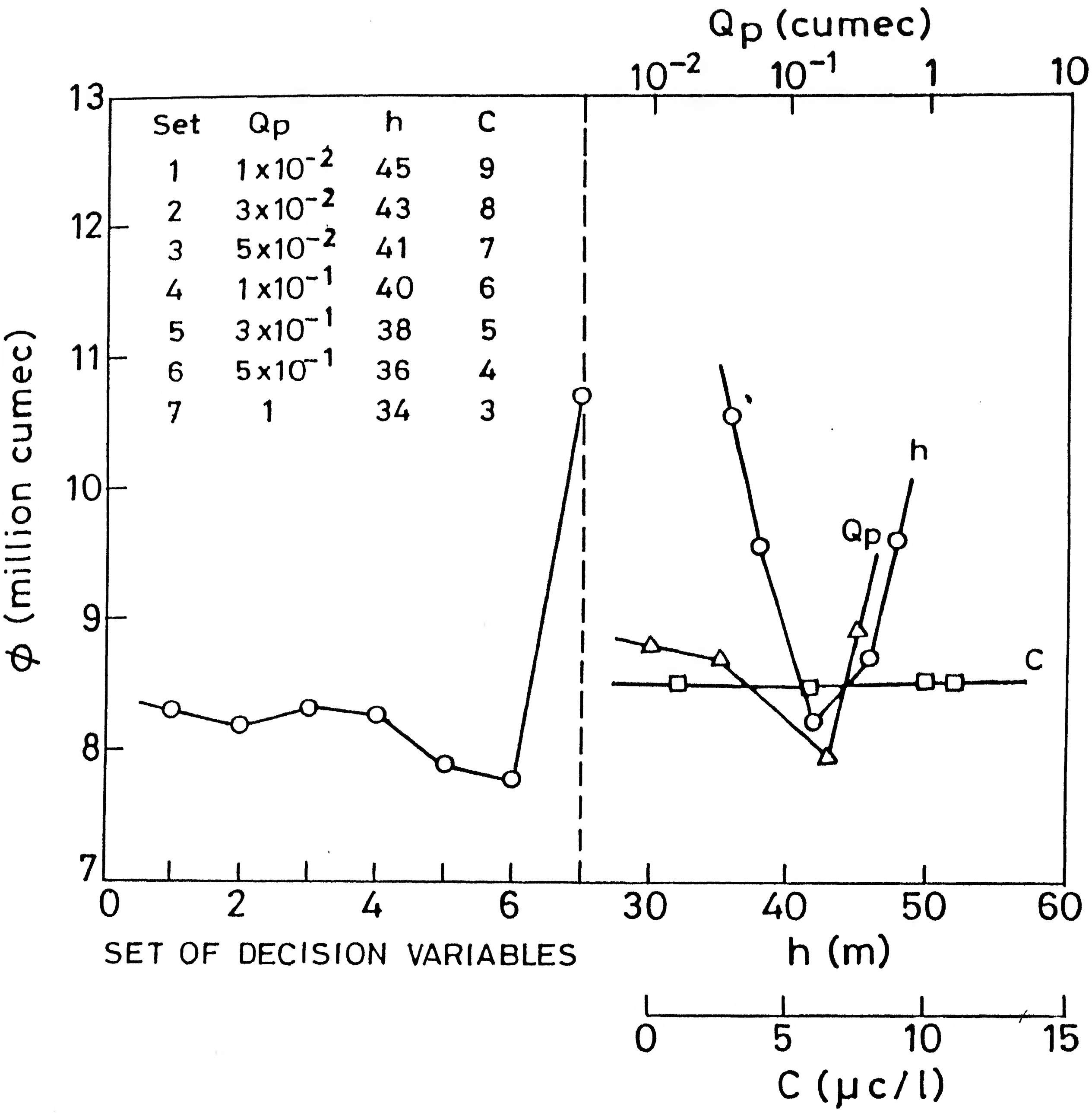
Table 6.3.7 Effect of variation in initial solution on optimal value for scenario 16

Initial solution set	Order of violation of simulation constraints		Objective function value	
$[\underline{h}, \underline{P}, \underline{C}]$	Flow	Transport	F	ϕ
[m, 1/s, μc/1]	(in S.I. unit)		(1/s)	(in S.I. unit)
[40, 50, 1]	$10^{-10}-10^{-12}$	$10^{-9}-10^{-11}$	4886.94	-3.9017
[40, 500, 1]	$10^{-9}-10^{-11}$	$10^{-9}-10^{-12}$	11320.12	-9.4681
[40, 5000, 1]	$10^{-10}-10^{-12}$	$10^{-9}-10^{-11}$	11087.22	-10.7469
[40, 5000,2]	$10^{-10}-10^{-12}$	$10^{-9}-10^{-12}$	11087.22	-10.4304

Fig. 6.3.9 shows the variation of composite objective function with decision variables at node (2,2) in first management period. It depicts that the function which is being minimized is nonconvex in nature. The large number of decision variables embedded in a complex manner in the composite objective function, and its different nature of affecting the system add to the complexity of identifying a global solution.

6.3.6 Summary

The methodology presented to solve the proposed integrated management model incorporating the coupled set of flow and advective -dispersive-diffusive-degradable transport equations is capable of solving the groundwater management problems in different natural and operational situations. The proposed management model which is generalized and applicable for conservative, radioactive and linear degradable pollutants need simple changes in the input structure to solve the various groundwater management problems dealing with these types of pollutants. The optimal solutions for different management scenarios are dependent on the boundary conditions, aquifer parameter estimates, impact of physical and natural processes and imposed managerial constraints. The optimal solutions for various management scenarios dealing with radioactive pollutant have similar characteristics as were discussed for conservative pollutants. However, the magnitudes of relative differences between solutions are of lesser order because of lesser pollutant load and



ig. 6.3.9 Variation of composite objective function with decision variabtes at node (2,2) in first management period.

comparatively low concentration gradient that exists in case of radioactive pollutant transport. The optimal solutions can be identified in less CPU time if better estimate is chosen as an initial solution vector. The global optimality problem no doubt arises in this case also.

SPECIAL CASE OF QUANTITY MANAGEMENT

SPECIAL CASE OF QUANTITY MANAGEMENT

In the previous sections, solutions of some groundwater gement models which incorporate the coupled set of flow and sport equations were presented and discussed. As a special case, aximization problem (Model I) which accommodates only the tity aspect is discussed in this section. The solution results his case will be helpful in those areas where either quality ct is not a limiting factor, or it is just ignored for lification. The management model for this case incorporates only ndwater flow equation as simulation constraints. This simulation tion in discretized form is incorporated in the management model sing the embedding technique. Thus, the composite objective tion consists of only F_1 and g_1 in this case. The model is uated for a number of management scenarios each representing erent boundary conditions, aquifer properties, and physical and managerial constraints. The outcomes of the model are the optimal pumping policies, and resulting spatial and temporal distribution of hydraulic heads. The global optimality of the solutions is also discussed along with the suitability and applicability of the developed model. Suitability of the implemented methodology to solve the groundwater management problems in different aquifer environment and operating conditions is also examined.

6.4.1 Description of the study area

Figs. 6.4.1a-6.4.1c show finite difference network for the

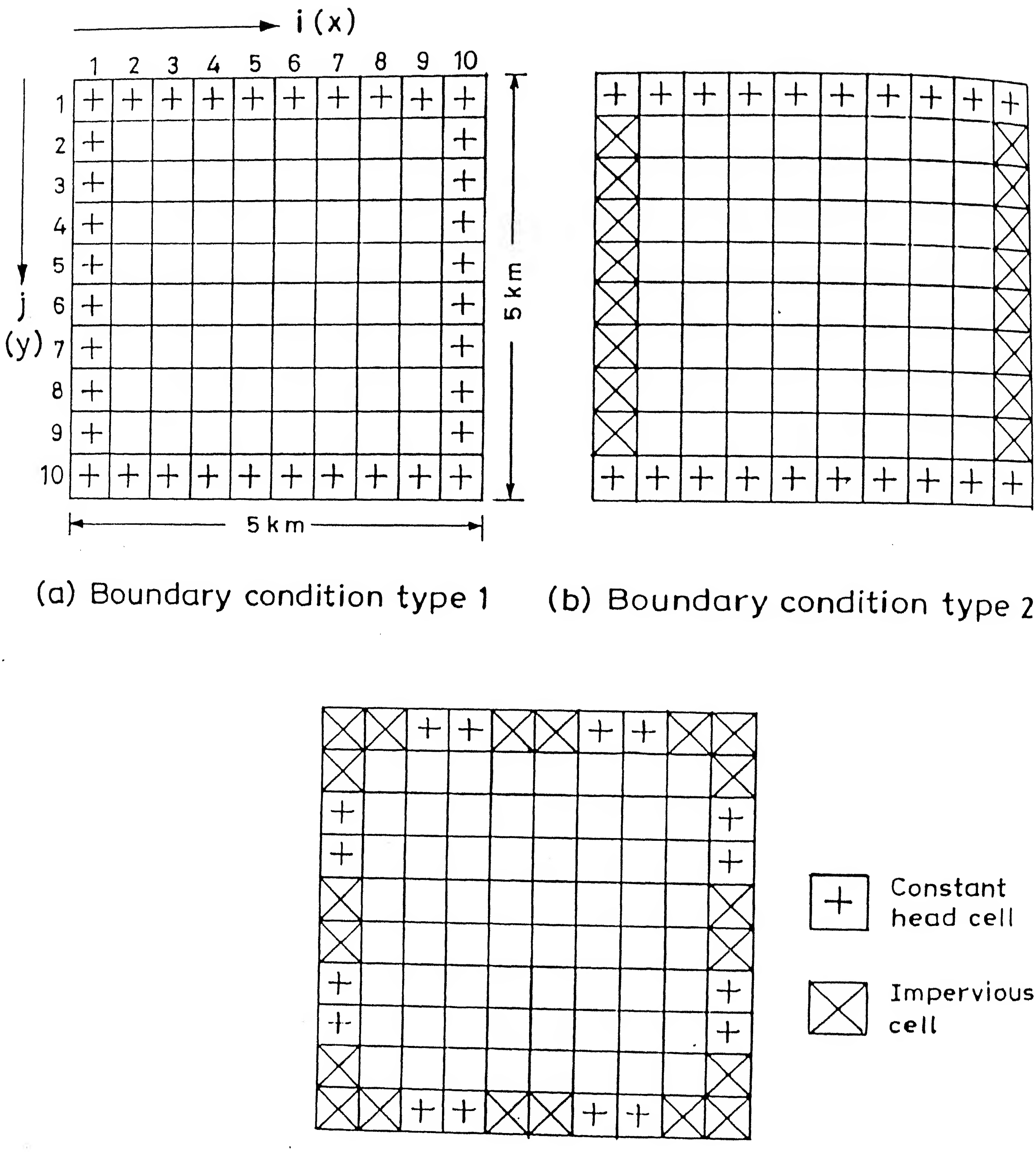


Fig.6.4.1 Finite difference network

study area of 2500 ha (5 km x 5 km) with different boundary conditions. The study area is divided into square cells, each of size 0.5 km x 0.5 km. The characteristic of management scenarios for which the model is evaluated are presented in Table 6.4.1. The aquifer is assumed homogeneous and anisotropic for the management scenarios 25-27 and 32-34. The management scenarios 28, 29 and 30 are based on the assumptions that the aquifer is respectively homogeneous and isotropic; heterogeneous and isotropic; and heterogeneous and anisotropic.

To illustrate the effect of heterogeneity and anisotropy, hydraulic conductivities for the scenarios 29 and 30 are estimated using exponentially varying deterministic expressions of the forms expressed by Equations 6.1 and 6.2. The values of K_o, a_{xx} (= a_{yx}) and a_{xy} (= a_{yy}) for scenario 29 are assumed 1.0×10^{-4} m/s, 0.23 km^{-1} and 0.18 km^{-1} respectively. The relative error in the mean value of computed hydraulic conductivities in this case is 0.07%. For the scenario 30, the values of K_o, a_{xx}, a_{xy}, a_{yx} and a_{yy} are assumed 1.0×10^{-4} m/s, 0.30 km^{-1}, 0.20 km^{-1}, 0.20 km^{-1} and 0.10 km^{-1} respectively. The relative errors in the mean values of computed K_{xx} and K_{yy} in this case are 0.73% and 0.37% respectively. Heterogeneous and anisotropic characteristic of the aquifer is also modeled using randomly generated spatial values of hydraulic conductivity (scenario 31). The hydraulic conductivity is assumed random in space following a Gaussian distribution with a standard deviation of 20% of the mean. The mean value in this case is 5.0e-04

Table 6.4.1 Description of management scenarios (Quantity aspect only)

Management Scenario	Type of Boundary Condition	Hydraulic Conductivity (m/sec) K_{xx}	K_{yy}	Leakage	Recharge	Lower Bounds on $\underline{h}$	$\underline{P}$	Upper Bounds on $\underline{h}$	$\underline{P}$
25	1	5×10^{-4}	4×10^{-4}	y	n	i	i	i	n
26	2	5×10^{-4}	4×10^{-4}	y	n	i	i	i	n
27	3	5×10^{-4}	4×10^{-4}	y	n	i	i	i	n
28	1	4.5×10^{-4}	4.5×10^{-4}	y	n	i	i	i	n
29	1	HEI		y	n	i	i	i	n
30	1	HEA		y	n	i	i	i	n
31	1	Random HEA		y	n	i	i	i	n
32	1	5×10^{-4}	4×10^{-4}	n	n	i	i	i	n
33	1	5×10^{-4}	4×10^{-4}	y	n	i	y	i	y
34	1	5×10^{-4}	4×10^{-4}	y	n	y	y	i	y

y exists
n does not exist
i inbuilt bound exists

HEI heterogeneous and isotropic
HEA heterogeneous and anisotropic

m/s for K_{xx} and 4.0e-04 m/s for K_{yy}. The relative error in the average values of both K_{xx} and K_{yy} (generated random data) is 1.42%.

The storage coefficient, effective porosity, thickness of leaky layer, saturated thickness of confined aquifer, hydraulic head in source bed and ground surface elevation are respectively 2.0e-04, 0.3, 2.0 m, 30.0 m, 55.0 m, and 62.0 m. These values do not change with respect to space and time. The vertical hydraulic conductivity of overlying leaky layer is 1.0e-12 m/s in all the management scenarios where leakage exists. Ten time frames are considered in a time horizon of five years.

In the top layer of boundary cells (Fig. 6.4.1), the hydraulic heads are specified as 50.0 m. In the bottom layer of boundary cells, the hydraulic heads are specified as 41.0 m. For the remaining cells, simple interpolation is used to obtain the head distribution. This distribution is considered as the specified initial hydraulic heads.

The inbuilt lower and upper bounds on hydraulic head variables are respectively the top of the confining layer and the ground surface. However, these inbuilt bounds can be made redundant by imposing more constraining managerial lower and upper bounds. The inbuilt lower bounds on pumping variables are zero and there is no inbuilt upper bound on pumping variables. The lower and upper bounds on pumping variables for scenarios 33 and 34 are estimated based on the irrigation demand from groundwater resource and capacity of available pumping equipments, respectively as explained in section

6.1.1. These bounds for each cell are respectively 15 l/s and 100 l/s throughout the planning period.

6.4.2 General discussion of results

Optimization runs are started with initial values of 40.0 m and 500 l/s for hydraulic head and pumping variables respectively. The values for ε_h and ε_q are taken 0.001 m and 0.01 l/s respectively. The starting step sizes are assumed 0.5 m for hydraulic head and 5 l/s for pumping variables. The optimal solutions for different management scenarios are summarized in Table 6.4.2. These results are obtained for $r = 10^{-18}$, $\alpha_q = \alpha_h = 2$, and $\beta_q = \beta_h = 1$. Table 6.4.2 gives the information about required CPU time, order of violation of flow equations, optimal total pumping, optimal value of composite objective function and number of function evaluations to obtain the optimal value for different management scenarios. The order of violation represents a magnitude equal to the product of a fractional number (< 1) with the values reported in this table. The yearly optimal pumping policies for different management scenarios are given in Table 6.4.3. It is evident from this table that yearly optimal pumping policy remains almost same throughout the planning period.

It is observed that this method is suitable for embedding technique which involves large number of variables and constraints to simulate the system. Investigation shows that even a larger sized study area for a large time span can be solved.

Table 6.4.2 Solution Results for management scenarios (Quantity aspect only)

Management Scenario	No. of Decision Variables	No. of Simulation Constraints	CPU Time (Min.)	No. of Function Evaluations	Order of Violation of Flow Constraints (in S.I. unit)	Optimal Total Pumping for 5-Yr. Planning Period (l/s)	Optimal Value of Composite Objective Function (in S.I. unit)
25	1280	640	91.64	122919	$10^{-9}-10^{-12}$	38848.49	-27.1098
26	1280	640	83.53	115236	$10^{-9}-10^{-12}$	18216.42	-17.7471
27	1280	640	84.75	115236	$10^{-8}-10^{-12}$	24078.88	-13.2313
28	1280	640	81.35	110114	$10^{-8}-10^{-12}$	40204.44	-23.3596
29	1280	640	84.05	112675	$10^{-8}-10^{-13}$	38001.34	-26.9937
30	1280	640	97.30	130602	$10^{-9}-10^{-13}$	41042.51	-39.6928
31	1280	640	91.74	122919	$10^{-9}-10^{-13}$	40388.32	-26.6073
32	1280	640	91.45	122919	$10^{-9}-0.0$	39469.04	-32.8200
33	1280	640	139.84	186944	$10^{-8}-10^{-12}$	18219.86	82.8406
34	1280	640	259.88	348287	$10^{-7}-10^{-12}$	15427.60	6.8879 $\times 10^4$

Table 6.4.3 Yearly optimal pumping policies for management scenarios (Quantity aspect only)

Management Scenario	Optimal pumping (l/s) in Management period (year)				
	1	2	3	4	5
25	7769.50	7769.74	7769.74	7769.74	7769.74
26	3644.54	3640.44	3640.44	3640.44	3650.52
27	4817.15	4815.42	4815.42	4815.42	4815.42
28	8041.71	8040.68	8040.68	8040.68	8040.68
29	7604.85	7599.12	7599.12	7599.12	7599.12
30	8210.08	8208.10	8208.10	8208.10	8208.10
31	8082.54	8076.44	8076.44	8074.44	8076.44
32	7910.73	7903.76	7903.76	7903.76	7847.00
33	3648.89	3640.48	3640.48	3640.48	3649.50
34	2275.06	2270.77	3624.70	3628.54	3628.54

The CPU time requirements for different scenarios presented in the Table 6.4.2 show that if decision space is more restricted by additional constraints, the CPU time required to solve the model increases appreciably (Scenarios 25, 33 and 34). This happens when the search goes in a undesirable direction because of imposed constraints. It makes the search length longer and more time is consumed to retrack the search process in a desirable direction. It should be noted here that any kind of change in the model, due to simplifications in the model or imposed constraints, results in a different optimal solution. If the time requirements and solution results are compared with those obtained for the integrated management models (Scenarios 11 and 12), the significance of quality aspect on computational requirements can be assessed. Inclusion of quality aspects renders the problem more complex and hence, CPU time requirement for solving will increase and optimal value of objective function will certainly change. This evidence also shows that comparatively a dimensionally large size problem can be solved more easily if only the quantity aspect is considered. The computation becomes relatively difficult when quality aspect is conflated in the model.

6.4.3 Effects of boundary conditions

To apply the model to a field problem, it is necessary to investigate the aquifer domain precisely. If proper boundary conditions are not assessed, the resulting optimal solution will not

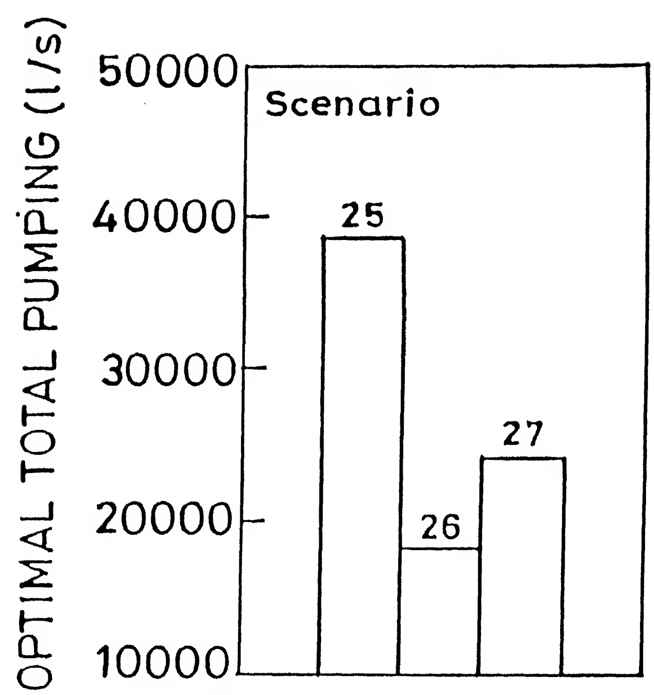


Fig. 6.4.2 Effect of specified boundary conditions on optimal total pumping

Table 6.4.4 Optimal pumping policy in fifth management period for scenario 25

	Optimal pumping (l/s)							
i →	2	3	4	5	6	7	8	9
j ↓								
2	539.06	251.34	158.61	160.57	188.91	190.96	210.82	517.46
3	202.62	193.91	150.04	121.70	127.07	140.08	166.09	189.88
4	141.68	143.73	29.92	270.70	283.98	46.52	149.61	152.68
5	161.41	76.02	25.70	25.94	26.04	29.20	65.14	148.69
6	113.44	102.19	25.62	256.24	256.24	27.83	56.72	115.14
7	134.88	111.25	27.19	25.62	25.62	34.96	113.85	145.98
8	145.27	123.71	95.35	39.06	55.29	77.93	140.64	136.84
9	175.16	147.75	116.15	108.96	109.04	123.24	128.44	148.50

Table 6.4.5 Optimal pumping policy in fifth management period for scenario 26

	Optimal pumping (l/s)							
i →	2	3	4	5	6	7	8	9
j ↓								
2	123.22	143.05	148.75	144.01	144.20	145.18	140.57	131.00
3	73.01	113.03	128.98	129.37	144.36	122.49	95.49	73.04
4	13.08	15.85	19.36	19.55	9.75	17.22	15.48	2.17
5	13.34	10.41	10.38	13.26	9.68	13.79	15.00	13.13
6	9.69	13.37	9.42	7.74	8.63	9.01	10.51	12.01
7	234.28	18.12	18.00	18.00	18.00	18.00	18.00	27.01
8	15.48	41.64	36.02	36.02	36.02	36.02	47.27	18.75
9	138.00	106.50	114.00	114.00	114.00	114.00	129.00	84.00

Table 6.4.6 Optimal pumping policy in fifth management period for scenario 27

	Optimal pumping (l/s)							
i →	2	3	4	5	6	7	8	9
j ↓								
2	157.23	179.96	159.20	64.10	71.35	147.95	164.26	167.25
3	128.44	154.65	103.07	43.11	54.28	92.17	153.48	133.50
4	145.43	66.91	23.61	17.79	17.40	19.10	113.26	171.00
5	74.43	32.60	13.77	13.77	14.24	16.27	52.68	137.71
6	67.62	17.64	13.77	13.77	13.77	19.78	21.86	101.35
7	116.46	48.09	17.13	17.87	17.56	24.94	31.62	100.14
8	101.82	121.33	51.43	26.23	31.05	34.10	79.18	144.37
9	117.01	130.74	51.66	45.06	43.32	53.81	96.39	140.62

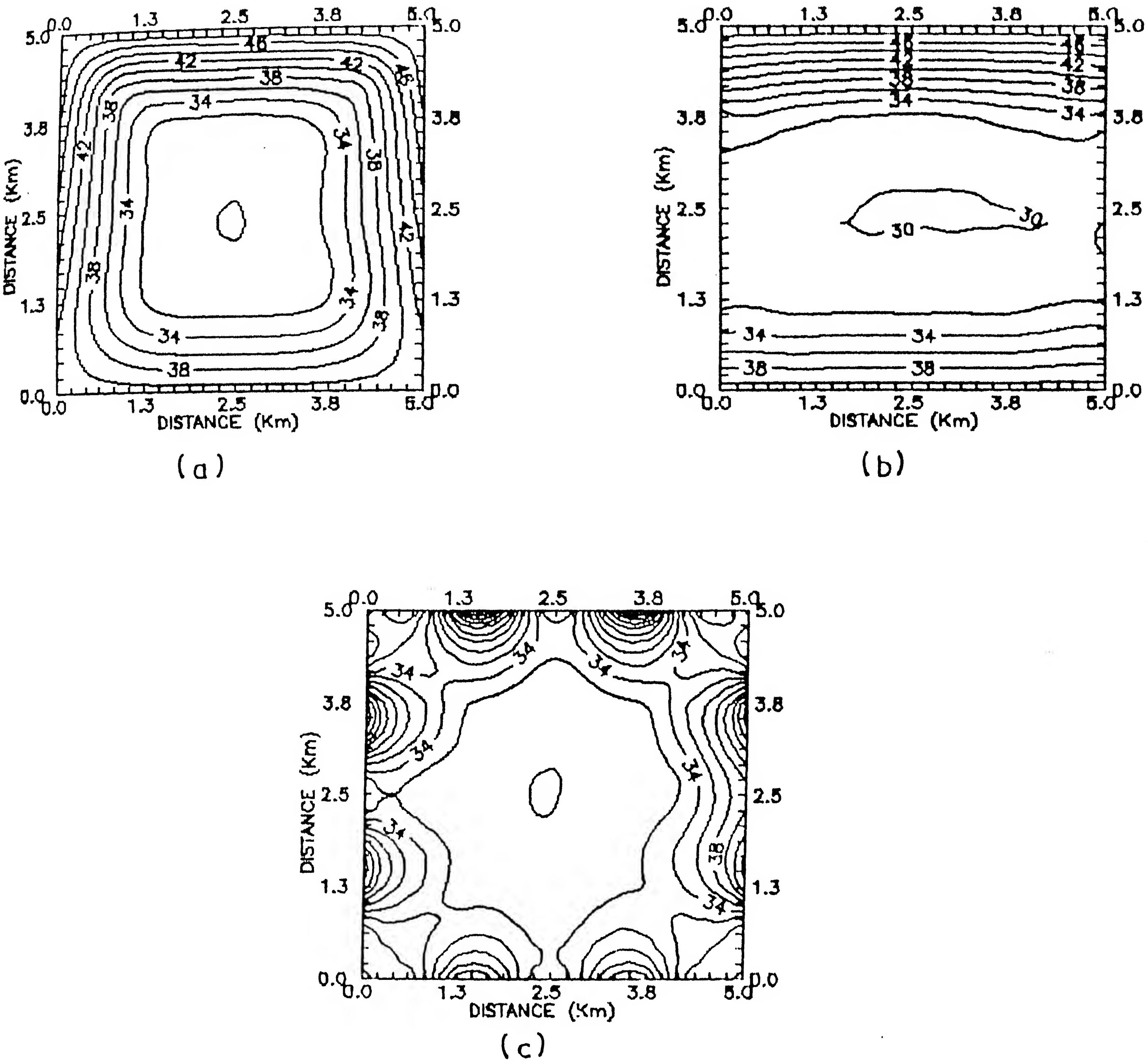


Fig. 6.4.3. Optimal spatial distribution of hydraulic head at the end of planning horizon for (a) scenario 25 (b) scenario 26 (c) scenario 27.

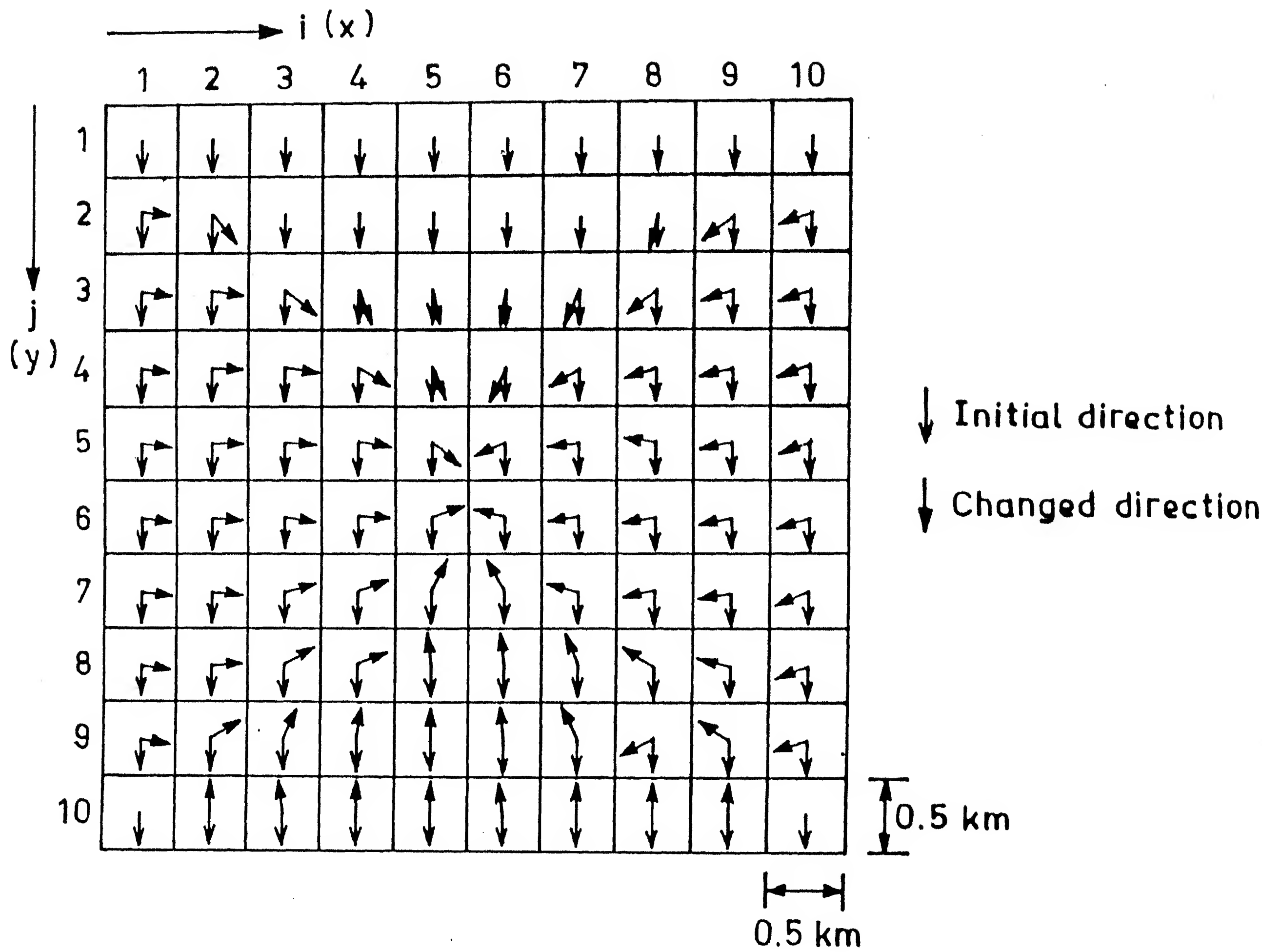


Fig. 6.4.4 Velocity field for scenario 25 in fifth year.

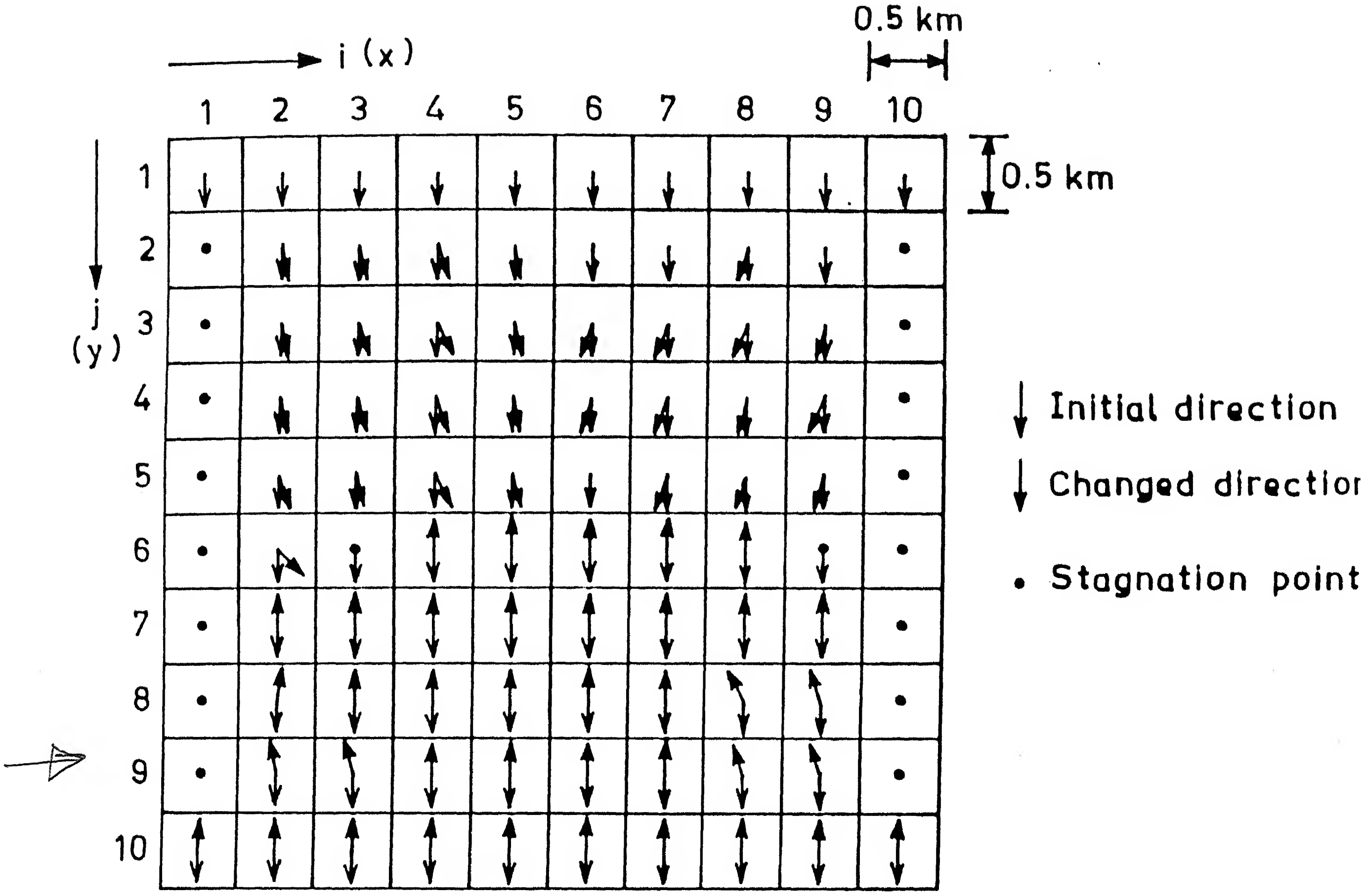


Fig. 6.4.5 Velocity field for scenario 26 in fifth year .

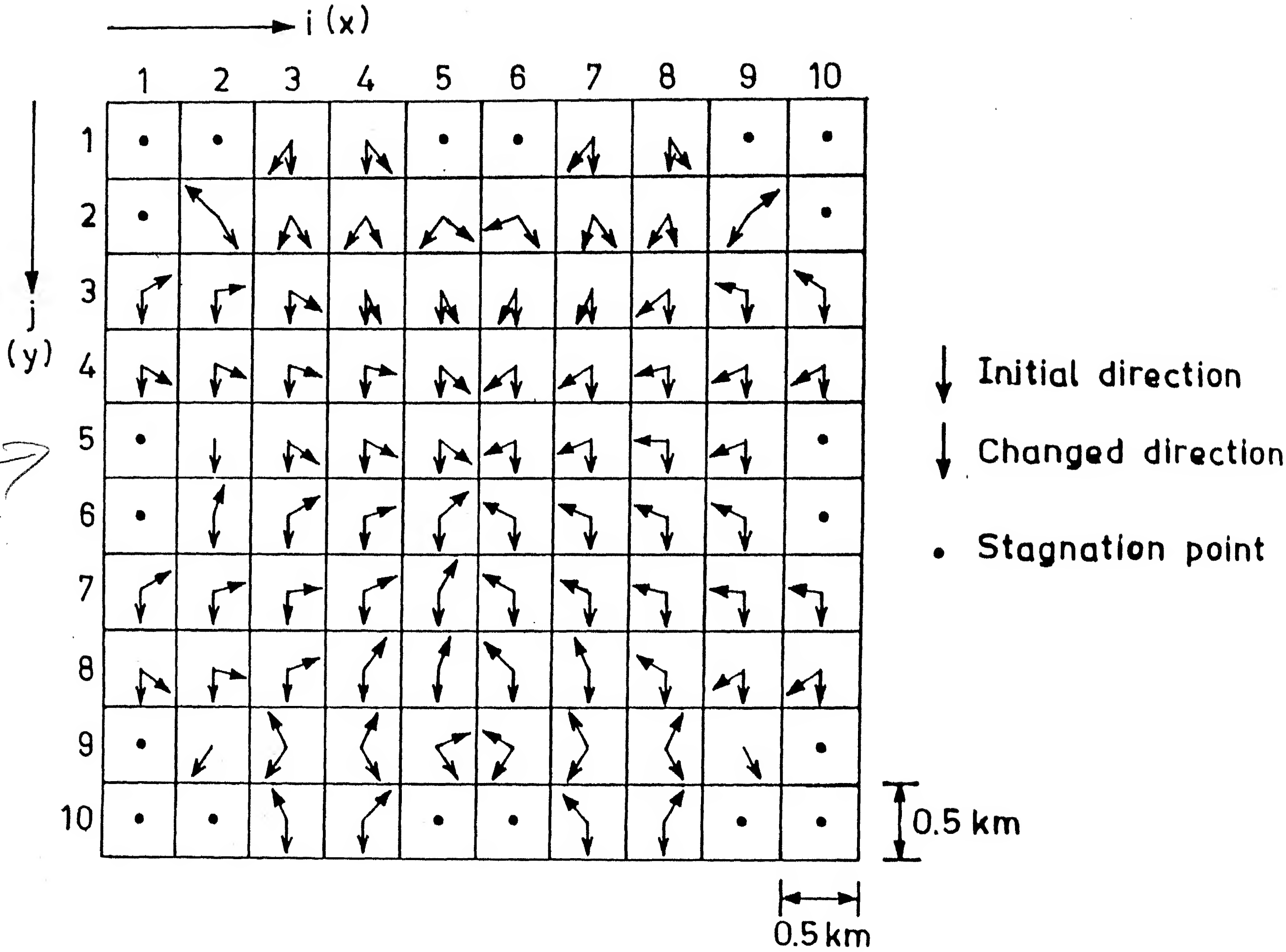


Fig. 6.4.6 Velocity field for scenario 27 in fifth year.

6.4.4 Effect of aquifer parameter estimates

Fig. 6.4.7 shows the effect of heterogeneity on optimal total pumping from isotropic and anisotropic aquifers. The anisotropy effect on optimal total pumping from homogeneous and heterogeneous aquifers is shown in Fig. 6.4.8. If the hydraulic conductivities are estimated by a randomized model instead of deterministic expressions, the resulting variation in the optimal total pumping is shown in Fig. 6.4.9. These results depict the dependence of optimal policies on the physical properties of the aquifer medium. Hence, accurate estimation of hydraulic conductivity plays an important role in optimal management. The same will be true for other aquifer parameter estimation also. However, for the results presented here, the change in total pumping is only about 5 % when the simplifying assumption of homogeneous and isotropic hydraulic conductivity is made. This effect will be more pronounced if the quality aspect is also taken into consideration or spatial variation of hydraulic conductivity is more in the real-life situations.

6.4.5 Effects of hydraulic head and pumping constraints

If the lower bound on hydraulic head is kept 40 m for the first and second management periods, 35 m for the third and fourth management periods and 30 m for fifth management period (Scenario 34), in addition to the imposed lower and upper bounds on pumping variables, the optimal total pumping and hence, yearly optimal pumping reduces appreciably. The impact of hydraulic head

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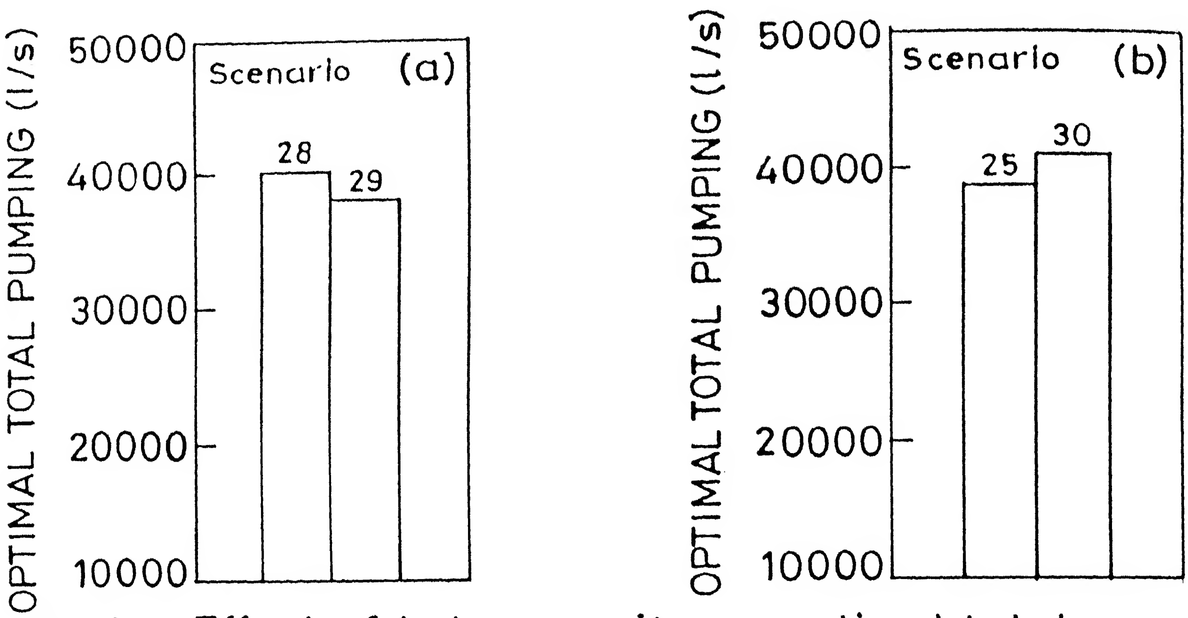

Fig. 6.4.7 Effect of heterogeneity on optimal total pumping from (a) isotropic aquifer (b) anisotropic aquifer.

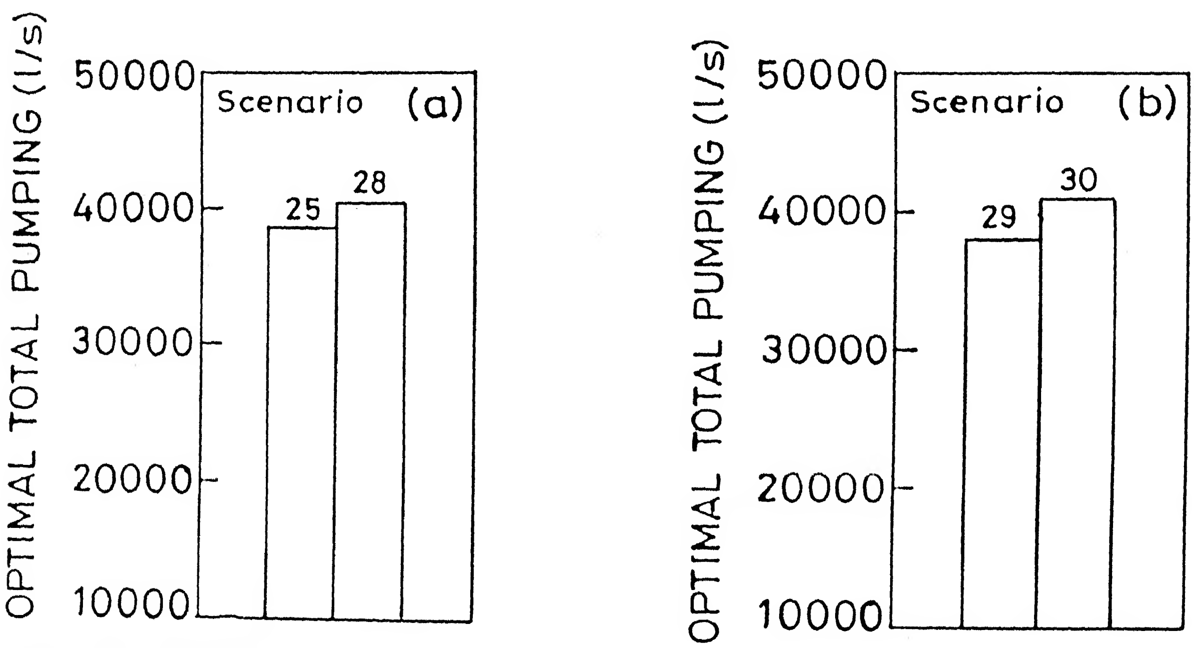

Fig. 6.4.8 Effect of anisotropy on optimal total pumping from (a) homogeneous aquifer (b) heterogeneous aquifer.

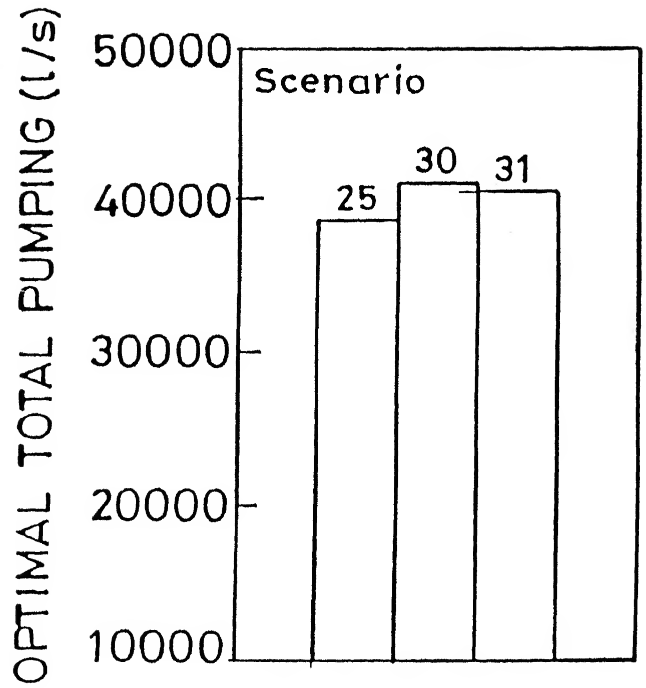

Fig. 6.4.9 Effect of deterministic and randomized modelling of hydraulic conductivity on optimal total pumping.

constraints on the optimal solution is shown in Fig. 6.4.10. Although yearly optimal pumping policy is reported in Table 6.4.3, the time step considered in the model is of six months duration. Therefore, all constraints and bounds must be satisfied for each of these time steps. The impact of pumping constraints on optimal total pumping is shown in Fig. 6.4.11. A comparison between the solutions for scenarios 25 and 33 shows that the optimal total pumping decreases when upper bounds on pumping variables are imposed on a cell by cell basis.

6.4.6 Global optimality of management strategies

The solution results obtained for different management scenarios can be guaranteed to be global only when an exhaustive number of optimization runs are made for each scenarios, each initiated with different sets of initial guesses. The optimal solution for each optimization run is picked up at the point of convergence. The problem of global optimality arises because of nonconvex nature of the composite objective function. Although, the simulation constraints of groundwater flow equations are linear in case of confined aquifer, the objective function becomes nonlinear if the exterior penalty function method is utilized to convert the constrained problem into unconstrained one. However, this problem will not arise if a linear solution technique, i.e. the Linear Programming (LP) algorithm is used. This problem of managing groundwater quantity aspect only is treated as a special case of the

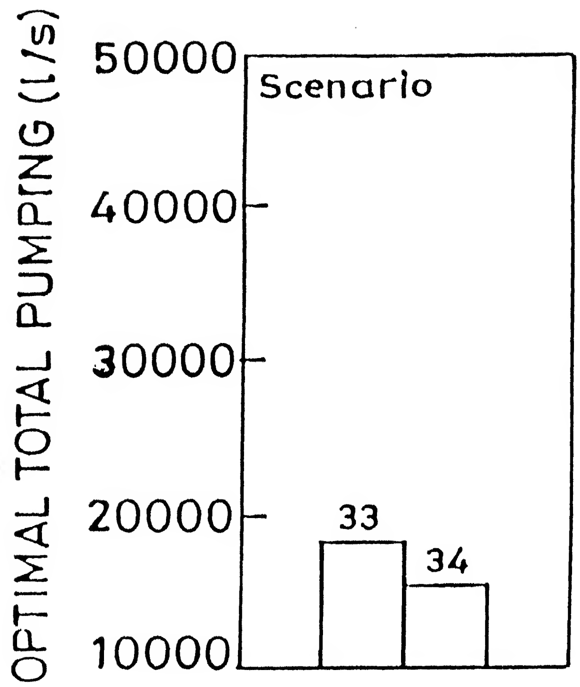

Fig.6.4.10 Effect of hydraulic head constraints on optimal total pumping.

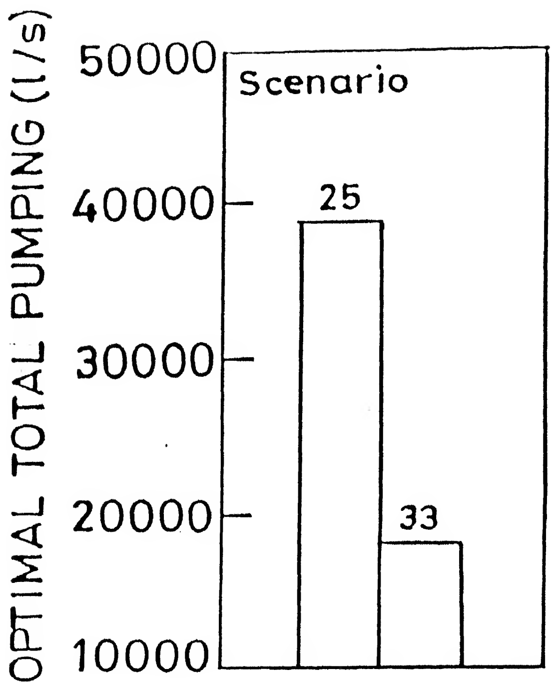

Fig.6.4.11 Effect of pumping constraints on optimal total pumping.

more generalized integrated management model. Therefore, the exterior penalty function approach is retained for solving this special case also. The variation of the composite objective function with different sets of initial guesses for decision variables is already discussed in Chapter 5. Therefore, this limitation also binds the applicability of the integrated management model to the management problems involving only linear constraints. This is a natural consequence of the solution methodology adopted.

6.4.7 Summary

The methodology presented here to solve the large sized multivariable constrained nonlinear groundwater management models can be applied to even larger sized multivariable constrained linear groundwater management models. However, global optimality problem may arise in case of nonconvex functions. The solutions obtained are no doubt very much dependent on the boundary conditions, physical and managerial conditions, aquifer parameter estimates, and certainly on given initial conditions. The optimal policies must be obtained with the proper aquifer parameter estimates and accurate inputs representing the real physical system. The models dealing with both quality and quantity aspects in a single framework are more difficult to solve and require more CPU time in comparison to the models dealing with only the quantity aspect.

COMPARISON OF IMPLEMENTED HJ AND PCD METHODS

CHAPTER 7

COMPARISON OF IMPLEMENTED HJ AND PCD METHODS

In the previous chapter, solution results of the proposed management models for various groundwater management problems dealing with different aquifer environment and operating restrictions were presented and discussed in detail. The solutions of the models were obtained using exterior penalty function method in conjunction with Hooke-Jeeves algorithm. The present chapter gives a detailed comparison between the implemented Hooke-Jeeves and Powell's conjugate direction methods used in conjunction with exterior penalty function approach to solve the developed groundwater management models. A brief theoretical comparison was also presented in Chapter 4. This chapter is devoted to the comparison between these two unconstrained methods of solution on the basis of solution results of groundwater management models. Some computational difficulties which arise during the implementation of these algorithms to solve the developed

groundwater management models, and their remedies are also described with proper explanation. The limitations of the proposed groundwater management models in terms of its applicability and the limitations of the results in terms of global optimality of the solutions are also discussed.

7.1 COMPARISON BASED ON SOLUTION OF THE MANAGEMENT MODEL

To compare the performance of implemented Hooke-Jeeves and Powell's conjugate direction methods, a maximization problem (Model I) for integrated management of quality and quantity aspects of a groundwater system as described in Chapter 3 is considered. The solutions of this maximization problem are obtained using both methods and the results are compared to assess the relative efficiency of these algorithms. Rate of convergence, CPU time and computer memory storage requirements are also discussed in the context of practical utility of the implemented algorithms. All computations are carried out on Convex/C-220 mini super computer system. Additional features of search procedure are also appended to give some insight to the search techniques.

7.1.1 Description of the study area

For simplification in terms of both computer memory storage and CPU time, 16-cell configuration each representing an area of 0.5 km x 0.5 km is considered as a finite difference network for 400 ha (2 km x 2 km) area with constant head boundary (Fig. 7.1). The model is

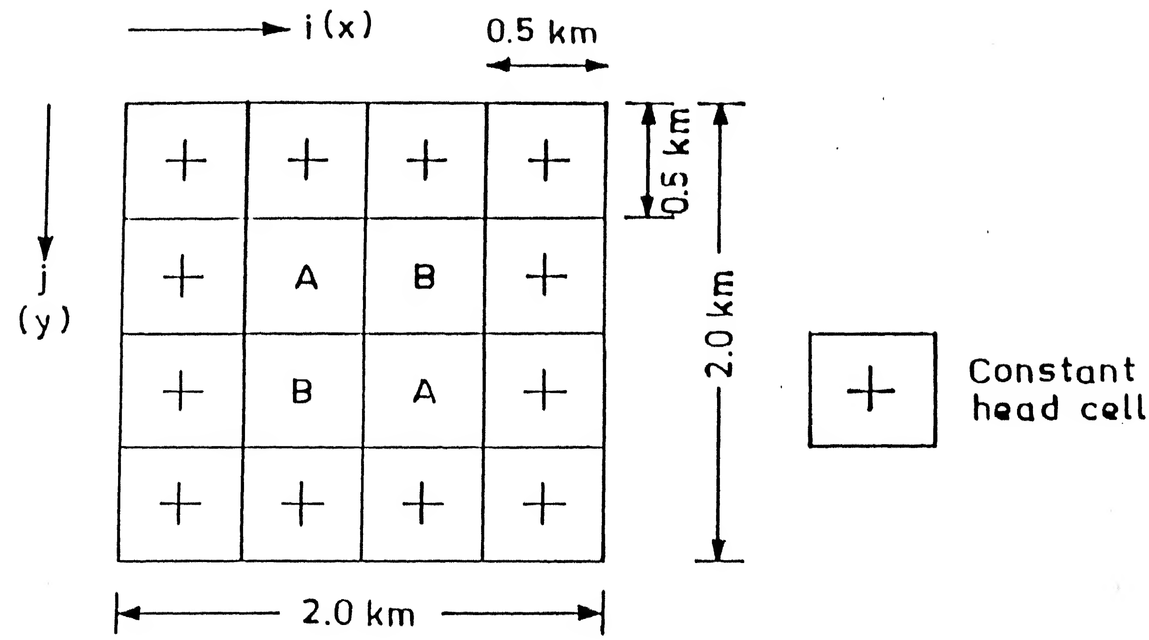

Fig. 7.1 Finite difference network.

applied to this study area to obtain the optimum solutions for a number of management scenarios using both the methods: (i) exterior penalty function method in conjunction with Hooke-Jeeves method (EPFM & HJ), and (ii) exterior penalty function method in conjunction with Powell's conjugate direction method (EPFM & PCD). The characteristics of the management scenarios are given in Table 7.1.

The aquifer system under consideration is assumed homogeneous and anisotropic. The hydraulic conductivities, K_{xx} and K_{yy} are respectively 5.0×10^{-4} m/s and 4.0×10^{-4} m/s. The storage coefficient, effective porosity, thickness of leaky layer, saturated thickness of confined aquifer, hydraulic head in source bed and ground surface elevation are respectively 2.0×10^{-4}, 0.3, 2.0 m, 30.0 m, 55.0 m and 62.0 m. These values do not change in space and time. The vertical hydraulic conductivity of overlying leaky layer is 1.0×10^{-10} m/s in all the management scenarios where leakage exists. There is no spatial variation of vertical hydraulic conductivity. The vertical point recharge in all the cells except boundary cells, when applicable is 1.0 l/s throughout the management period. The recharge at all boundary cells is assumed zero. The solute considered here is chloride, a conservative pollutant. The concentration of chloride entering the internal cells denoted by A and B (Fig. 7.1) are respectively 200 mg/l and 100 mg/l in recharge, and 150 mg/l and 100 mg/l in leakage. The longitudinal and transverse dispersivities are 30 m and 10 m respectively. Two time frames are considered in a time horizon of two years. However, the

Table 7.1 Description of management scenarios

Management scenario	Hydraulic Conductivity (m/sec) K_{xx}	K_{yy}	Leakage	Recharge	Lower Bounds on $\underline{h}$	$\underline{P}$	$\underline{C}$	Upper Bounds on $\underline{h}$	$\underline{P}$	$\underline{C}$
35	5×10^{-4}	4×10^{-4}	n	n	i	i	i	i	n	n
36	5×10^{-4}	4×10^{-4}	y	n	i	i	i	i	n	n
37	5×10^{-4}	4×10^{-4}	y	y	i	i	i	i	n	n
38	5×10^{-4}	4×10^{-4}	y	y	i	y	i	i	y	n
39	5×10^{-4}	4×10^{-4}	y	y	i	y	i	i	n	y

y exists
n does not exist
i inbuilt bound exists

solution can be obtained in the same manner for more time frames. Again, less number of time frames are considered only for simplicity in terms of computer memory storage and CPU time requirement to achieve an optimal solution.

In the top layer of boundary cells (Fig. 7.1), the hydraulic heads are specified as 50.0 m. In the bottom layer of boundary cells, the hydraulic heads are specified as 44.0 m. For the remaining cells, simple interpolation is used to obtain the head distribution, which are considered as the specified initial heads. Existing concentrations at all boundary cells are specified as zero. The initial concentration in the aquifer for the cells denoted by A and B (Fig. 7.1) are 500 mg/l and 300 mg/l respectively.

The inbuilt lower and upper bounds on hydraulic heads are respectively the top of the confining layer and the ground surface. However, these inbuilt bounds can be made redundant by imposing more constraining managerial lower and upper bounds. The lower bounds on pumping variables for scenarios 38 and 39 are determined on the basis of agricultural requirement. The upper bounds on pumping variables at each cell are estimated on the basis of capacity of maximum two pumps each of 80 H.P. with assumed efficiency of 65 percent (scenario 38). These bounds for each cell are estimated as discussed in Chapter 3. Thus, lower and upper bounds on pumping variables become respectively 15 l/s and 200 l/s throughout the planning period. In case of inbuilt bounds where these constraining bounds do not exist, the inbuilt bounds specify nonnegativity as

lower bounds and none for upper bounds. For the concentration variables, the lower bounds are generally specified to be zero to have nonnegative values, while upper bounds imposed for scenario 39 are 250 mg/l. There is no inbuilt upper bound on concentration.

7.1.2 Optimal solutions of the management scenarios

The model is solved for different management scenarios using both methods. All optimization runs are started with a initial solution set having the values of 40 m for hydraulic head variables, 50 l/s for pumping variables and 100 mg/l for concentration variables. The value of penalty parameter used in the computation is 10^{-18}. In case of HJ method, the values of other optimization parameters are taken as $\alpha_h = \alpha_q = \alpha_c = 2$, $\beta_h = \beta_q = \beta_c = 1$, ε_h = 0.001 m, ε_q = 0.01 l/s and ε_c = 0.01 mg/l. The initial step sizes are assumed as Δh = 0.5 m, Δq = 5 l/s and Δc = 10 mg/l. The values of ε_{1dv}, ε_{1df}, ξ_h, ξ_q, ξ_c, $d\xi_h$, $d\xi_q$ and $d\xi_c$ required in PCD method to solve the model are assumed 0.3, 0.3, 0.5, 0.005, 0.01, 0.05, 0.0005, and 0.005 respectively. All these values correspond to the computations performed in S.I. units. To terminate the execution in PCD method, the value of 'ntermi' is taken as 1626 (65 cycles) for scenarios 35 and 36, and 1751 (70 cycles) for scenarios 37, 38 and 39.

The optimal solutions of different management scenarios, obtained from both methods (EPFM & HJ) and (EPFM & PCD) are tabulated in Table 7.2 for comparison. This comparison shows that the optimal

Table 7.2 Optimal solutions for management scenarios

Management scenario	Method	Optimal total pumping (l/s)	Composite objective function (in S.I. unit)	Order of violation of simulation constraints (in S.I. unit)	
				Flow	Transport
35	EPFM & HJ	675.20	- 0.5768	$10^{-10}-10^{-11}$	$10^{-9}-10^{-10}$
35	EPFM & PCD	691.90	- 0.6918	$10^{-11}-10^{-12}$	$10^{-11}-10^{-12}$
36	EPFM & HJ	599.72	- 0.5776	$10^{-10}-10^{-12}$	$10^{-10}-10^{-11}$
36	EPFM & PCD	685.26	- 0.6841	$10^{-10}-10^{-12}$	$10^{-8}-10^{-12}$
37	EPFM & HJ	584.94	- 0.5836	$10^{-10}-10^{-12}$	$10^{-10}-10^{-11}$
37	EPFM & PCD	771.30	- 0.7319	$10^{-10}-10^{-11}$	$10^{-9}-10^{-11}$
38	EPFM & HJ	587.00	- 0.5859	$10^{-10}-10^{-12}$	10^{-11}
38	EPFM & PCD	750.29	46.3730	$10^{-10}-10^{-12}$	$10^{-8}-10^{-11}$
39	EPFM & HJ	1052.30	32.60	$10^{-9}-10^{-11}$	$10^{-8}-10^{-9}$
39	EPFM & PCD	1132.90	62.26	$10^{-8}-10^{-12}$	$10^{-8}-10^{-9}$

solutions representing total pumping obtained from the Powell's conjugate direction method are better than those obtained from the Hooke-Jeeves method. The optimal values obtained from these two methods are similar in magnitudes. These observations also establish the validity of both the implemented algorithms to solve the nonlinear groundwater management models. In all the scenarios considered, the optimal solutions show improvements in PCD method. Solutions from both methods for all scenarios are obtained by using identical initial guesses to facilitate comparison.

These results show that PCD method is more efficient in obtaining the optimal solution. The number of iterations allowed is not a limitation in either of the two methods tested. For scenarios 37 and 38, the optimal total pumping obtained from PCD method is appreciably more in comparison to that obtained from HJ method. It is concluded that the PCD method will in general give better result compared to the HJ method, although in some cases, the difference may be marginal. This evidence is more clear from Fig. 7.2 as all the points fall below the 1:1 line.

7.1.3 Rate of convergence

To see the convergence of the PCD and HJ methods, the composite objective function values at every cycle (in PCD method) or iteration (in HJ method) for all the scenarios are plotted in Figs. 7.3 and 7.4 respectively. It is evident from these figures that the improvement in the value of composite objective function is more in

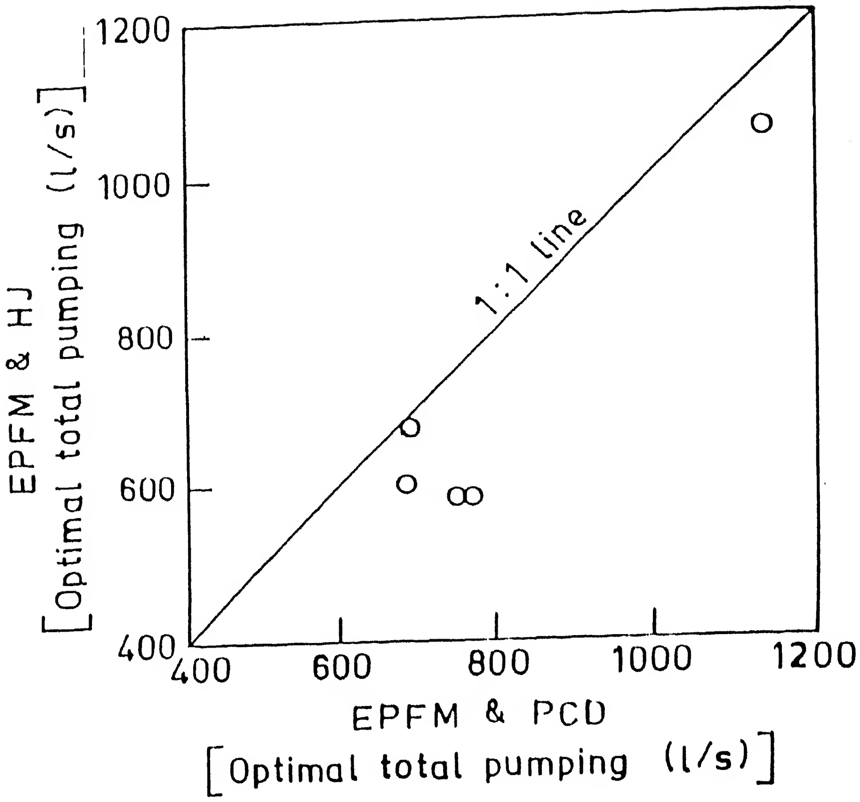

Fig. 7.2 EPFM & PCD vs. EPFM & HJ.

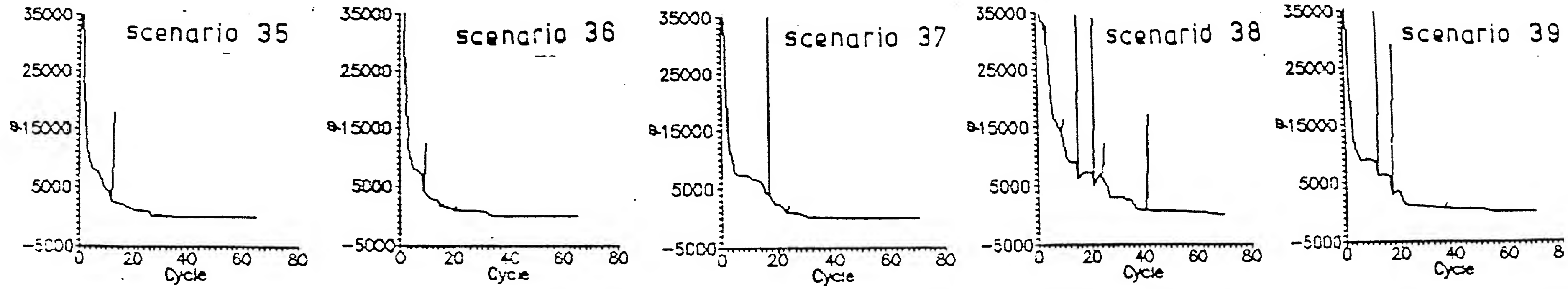

Fig. 7.3 Variation of composite objective function with number of cycles in PCD method.

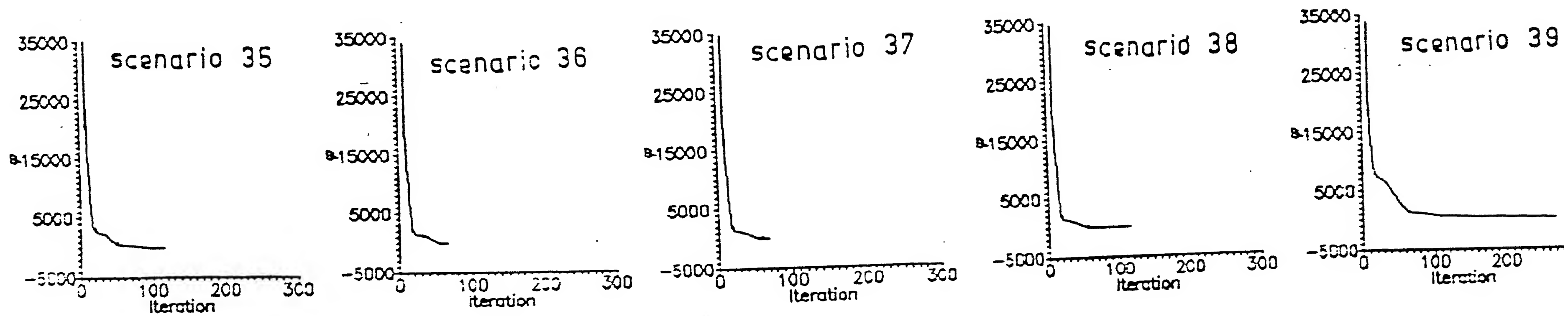

Fig. 7.4 Variation of composite objective function with number of iterations in HJ method.

case of PCD method after one cycle, when compared with that of the HJ method after one iteration. Thus, rate of convergence of the implemented PCD method is more than that of implemented HJ method.

7.1.4 CPU time and memory storage requirements

The CPU time requirements on a Convex/C-220 mini super computer system for solving the integrated management model using HJ and PCD methods in conjunction with exterior penalty function method for various scenarios are given in Table 7.3. This comparison shows that in case of PCD method, function is evaluated large number of times to obtain the optimal solution. Thus, CPU time requirement in PCD method is comparatively more than that in HJ method (Table 7.3). It happens because computation of objective function value is a time consuming activity especially when quality aspect is coupled with the quantity aspect in modeling. Although, the rate of convergence is more in case of PCD method as discussed in section 7.1.3, the CPU time requirement is more because large number of function evaluations are involved. This is an inherent property of this methodology as there is no pattern move similar to the HJ method in the PCD method. In the PCD method, in every cycle, the search is made like exploratory search of HJ method with a new direction set, e, obtained in a manner similar to the pattern move.

The demerit of PCD method is that it needs a large memory space for storing the direction vector. For example, even for 36-cell configuration (16 internal cells with three different classes of

Table 7.3 CPU time requirements for various management scenarios

Management scenario	Number of function evaluations		CPU time (Minute)	
	EPFM & HJ	EPFM & PCD	EPFM & HJ	EPFM & PCD
35	6213	23833	18.65	75.98
36	3714	24080	11.36	76.89
37	3910	30023	11.90	85.00
38	6115	54111	18.40	171.52
39	1371	25527	40.00	82.00

decision variables), the space needed to store the direction vector is 57840 bytes if only five time steps are considered. The code contains two such variables and thus needs approximately 0.12 Megabytes in addition to the space needed for other variables. This space is not needed in case of the HJ method. Therefore, the computer memory storage requirement is much less in case of HJ method as compared to PCD method.

7.1.5 Some additional salient features of search

Some additional salient features of the search processes performed to obtain the optimal solutions for various scenarios are enumerated in Tables 7.4-7.7. Table 7.4 provides the information about the number of exploratory search failures, number of pattern search failures and number of increment reductions for step sizes, which are the characteristics of the search procedure of the implemented HJ algorithm. The number of infeasible pattern moves for pumping, hydraulic head and concentration variables that occurred during the course of optimization for various scenarios using this methodology are listed in Table 7.5. These values are shown only for those iterations in which such infeasible pattern moves have occurred.

Table 7.6 shows the number of one dimensional searches and number of inefficient conjugate direction sets which are encountered during the optimization with Powell's conjugate direction method for different scenarios. The number of infeasible direction moves for

Table 7.4 Search abstract for various management scenarios (HJ method)

Scenario	Number of exploratory search failures	Number of pattern search failures	Number of increment reductions for		
			Δq	Δh	Δc
35	11	11	9	9	10
36	11	11	9	9	10
37	11	11	9	9	10
38	11	11	9	9	10
39	11	11	9	9	10

Table 7.5 Infeasible pattern moves during optimal search for various management scenarios (HJ method)

Iteration No.	Scenario 35			36			37			38			39		
	Number of infeasible pattern moves for														
	h	p	c	h	p	c	h	p	c	h	p	c	h	p	c
10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
18	0	0	1	0	0	0	0	0	0	0	0	0	0	0	1
19	0	0	0	0	0	1	0	0	1	0	0	1	0	0	1
21	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
22	0	0	0	0	0	1	0	0	1	0	0	1	0	0	1
24	0	0	0	0	0	1	0	0	1	0	0	1	0	0	0
26	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
50	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
57	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0
60	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
61	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
63	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
65	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0
74	0	0	0							0	1	0	0	0	0
76	0	0	0							0	0	0	0	1	0
78	0	0	0							0	1	0	0	1	0
79	0	0	0							0	0	0	0	1	0
83	0	0	0							0	1	0	0	0	0
84	0	1	0							0	0	0	0	0	0
103	0	0	0							0	1	0	0	0	0
109	0	0	0							0	1	0	0	1	0
119													0	1	0
148													0	1	0
162													0	1	0
163													0	1	0
269													0	1	0

Table 7.6 Search abstract for various management scenarios (PCD method)

Scenario No.	Number of one dimensional searches	Number of inefficient conjugate direction sets
35	1634	8
36	1633	7
37	1757	6
38	1759	8
39	1759	8

Table 7.7 Infeasible direction moves during optimization for various management scenarios (PCD method)

Scenario	Number of infeasible direction moves for		
	<u>h</u>	<u>P</u>	<u>C</u>
35	0	142	100
36	0	170	75
37	0	152	185
38	0	547	68
39	0	331	208

pumping, hydraulic head and concentration variables that occurred during the course of optimization for various scenarios using this methodology are given in Table 7.7. These values are tabulated on the basis of those stages in which such situations have occurred.

The salient features presented here provide insight to the working procedure of the implemented algorithms used for solving the groundwater management models. These details are appended to illustrate the progress of search processes to obtain optimal solution of the management model for any particular scenario.

7.2 SOME COMPUTATIONAL DIFFICULTIES AND THEIR REMEDIES

During the development of the optimization code (NLOGM) for solutions of the groundwater management models in different aquifer environment and operational situations, some computational difficulties are encountered. These difficulties are described in the following subsections. To overcome these difficulties, suitable remedial measures are adopted. The explanation of these adopted remedies are also discussed to justify their use.

7.2.1 Stagnation point

The stagnation point represents the cell, node, or any point where velocity becomes zero. The stagnation point problem arises when dispersion coefficients are computed at these points or cells where velocity is having zero value. The zero velocity at such points makes the dispersion coefficients indeterminate. It may occur

at a point or a cell because of equal flow towards the point or cell from the coordinate directions. Generally, this problem is frequently encountered at the beginning of the search if initial guesses for all hydraulic head variables are same or initial guesses are such that velocity in some cells possess a zero value.

To eliminate the stagnation point problem at the beginning of the search process which is a consequence of the initial guesses for hydraulic head variables, the initial guesses are perturbed by a very small amount to yield no absolute stagnation point in the aquifer domain. Perturbation by a very small amount, 10^{-9} m for example, gives nonzero velocity all over the aquifer domain. However, for simplification, it is advisable to increment the initial guesses for hydraulic head variables of each layer of cells by 10^{-3} m row wise or column wise to ensure either vertical or horizontal nonzero velocity. This does not introduce any error in the result because initial guesses may be any value, even infeasible.

If the stagnation point arises because of zero resultant flow in the intermediate stages of the search processes, the velocity at this point is made nonzero by a very small amount, may be in the order of 10^{-12} m/s. The contribution of this negligible velocity towards the dispersion coefficients may be regarded as the effect of molecular diffusion.

7.2.2 Inverted 'L'

Inverted 'L' represents the corner cells where a set of impermeable or no flow cells have a shape of an inverted 'L'. This is shown in Fig. 7.5. Such situations may occur at only one or more than one corners. This type of boundary condition makes these cells stagnant. Again, in such type of cells, the dispersion coefficients become indeterminate. To overcome such type of problem, the impermeable cells are assumed to have negligible hydraulic conductivities, may be of the order of 10^{-14} m/s. This remedial measure is necessary for other cells also, which are impermeable or no flow types. Mixed type boundary conditions which result in inverted 'L' problem, together with associated solution results are discussed in Chapter 6. The variations in dispersion coefficients resulting from this remedial measure may be regarded as the effect of molecular diffusion. Although, molecular diffusion has been otherwise neglected in the solution of the models, its small contribution in these special cases are not significant and hence, obtained optimal solutions are not affected significantly.

7.2.3 INF and NAN in SQEM

INF and NAN signify two different error criteria encountered during the execution of a computational code. INF represents an infinity problem which may arise in successive quadratic estimation method during the finding of optimal step length in one dimensional search of the PCD algorithm. NAN represents the occurrence of '0/0'

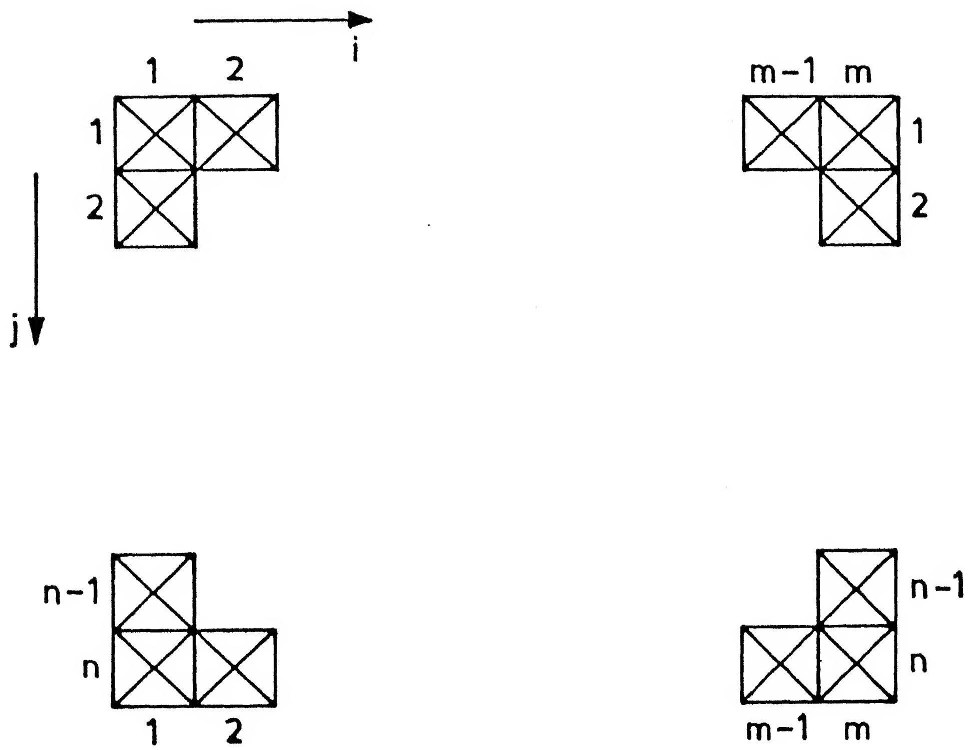

Fig. 7.5 Inverted 'L' at corners of aquifer domain.

change the search direction, but deviation from the actual optimal solution of the model will be generally insignificant. This is because such situations will occur only when ξ_1, ξ_2 and ξ_3 are very close to each other or when such situations are forced because of imposed managerial constraints, as explained in Chapter 4.

This problem also arises when search directions become linearly dependent. It generally occurs whenever the optimal step length in any particular direction happens to be zero. The PCD method can simply come to a halt before reaching the minimum point because of dependent search directions in the course of numerical computation. Due to linear dependency, the direction vector becomes sparse. However, this problem is eliminated by incorporating the above mentioned modifications together with the modifications discussed in Chapter 4.

7.2.4 Scaling

The integrated management model developed in this thesis does not suffer severly from the scaling problem, because order of magnitude of all simulation constraints expressed by finite difference forms of groundwater flow and solute transport equations are almost similar or comparable. They do not differ from each other drastically. However, scaling problem may arise between constituent terms within a constraint because of the values of decision variables involved, during the optimization process.

The enormous difference in scale between decision variables due

to difference in dimensions may also cause some difficulties in selecting step length, termination parameters or other optimization parameters depending upon the method employed for calculating numerical derivatives. Sometimes the objective function (composite objective function in constrained problems) contours may distort due to these scale disparities which will make the problem progressively ill-conditioned. This problem has been eliminated by defining different values of retardation factors, acceleration factors, termination parameters and initial step sizes for different classes of decision variables in HJ method; and by using different values for initial guesses and step sizes for the different classes of decision variables in one dimensional search in PCD method. Due to nongradient based techniques used, the difficulties in computing numerical derivatives do not arise. Therefore, possibility of severe scaling problem is scarce. The model may be made more robust by nondimensionalizing all decision variables involved in objective functions and constraints.

7.2.5 Curse of dimensionality

Curse of dimensionality is the inherent and most severe problem hindering the widespread application of nonlinear programming. However, the HJ algorithm for the solution of groundwater management models is affected to a lesser degree by this problem. In PCD algorithm, dimensionality problem may become more acute for very large sized study areas involving a large number of decision

variables. Basically this problem should be discussed in conjunction with the capability of the computers available for computing, especially in terms of speed and available storage. It is felt that comparatively low speed computers such as HP 9000/850 super mini computer system is affected by dimensionality problem especially when used in time sharing environment. This computer system requires a large CPU time to obtain the optimal solution, however, storage is not a problem. The CPU time requirement is less of a problem in case of high speed computers like Convex/C-220 and HP 9000/735 even when used in time sharing environment. It is observed that CPU time required by HP 9000/850 computer system is approximately 1.70 times that required by Convex/C-220 computer system. Storage requirement is not a hindrance for main frames if a dedicated system is available. Therefore, wide applicability of nonlinear programming depends upon the availability of high speed computers and the prospects will certainly improve with the advent of such computers having more and more speed and storage space.

7.3 MODEL LIMITATIONS AND GLOBAL OPTIMALITY

All the developed models described in this study are applicable to those groundwater management systems where the assumptions outlined in Chapter 3 are not violated. However, slight modifications in the developed codes can incorporate many other field situations and will be applicable to a variety of field problems. It should be noted here that the applicability of the

model is illustrated through the problems in which molecular diffusion contribution has been neglected in general. However, in order to accommodate some computational remedial measures for second and third type of boundary conditions, negligible contribution of molecular diffusion has been incorporated. The developed model with minor modifications in the computation of dispersion coefficients can be applied to the problems in which either molecular diffusion is significant or predominant. These models are not applicable for adsorbed and chemically reactive pollutants. Incorporation of these phenomena requires only slight modifications in the models. To apply the code (NLOGM) for other types of boundary conditions not discussed here, some modifications are required in the computer code.

No doubt, the usability of the present methodology also is limited by its inability to guarantee global optimality of the solutions. This problem is common in most engineering problems because of involved nonlinearity and nonconvexity of the objective function and the decision space. To overcome this, an exhaustive number of local optima must be identified to establish the global optimality of a solution. This remains the most challenging problem and further research is essential to either devise a strategy to find global solution or to reduce the number of searches for a global optimal solution.

7.4 SUMMARY

The comparison between the implemented HJ and PCD methods in conjunction with exterior penalty function method to solve groundwater management models is presented in this chapter. These comparisons are based on solution results for different management scenarios and theoretical basis of the search procedures. The efficiency, suitability, convergence, CPU time requirement, computer memory storage requirement and some additional features of search procedures are discussed and compared. It is observed that PCD method is more accurate, but HJ method is more robust, versatile, and computationally feasible. Thus, selection of a particular method relies on the nature of the problem, accuracy desired, and availability of the computing power. Some computational difficulties encountered during the development of the code for these algorithms and their remedies are also discussed. Finally issues related to the limitations of the model and global optimality of the solutions are discussed. The following chapter will focus on the extension of the model and methodology to incorporate multiple objectives of planning and management.

EXTENSION TO MULTIOBJECTIVE MANAGEMENT PROBLEMS

CHAPTER 8

EXTENSION TO MULTIOBJECTIVE MANAGEMENT PROBLEMS

The groundwater management models discussed in the previous chapters and applied to various groundwater problems involve only single objective. In many real-life situations involving management of groundwater resources, more than one objective is involved. These objectives may be of conflicting nature. Optimum management policies for the problems involving conflicting objectives can not be obtained by decomposing the multiple objectives into single objective optimization problems without taking into account the interdependability and then solving it. Nonconflicting objectives can be combined into a single objective and thus, transform a vector optimization problem into a scalar optimization problem. Such transformations are not possible for conflicting objectives.

Management problems involving conflicting objectives are solved by multiobjective optimization techniques. Such problems frequently

occur in the regional planning and operation of groundwater systems for various purposes. An example of a two conflicting objectives problem is to maximize the pumping and also to minimize the cost of pumping. This chapter is devoted to deal with the description, formulation and solution of the multiobjective management problem. To illustrate the solution procedure, the management model is formulated as a two objective groundwater management model involving groundwater withdrawal and groundwater pollution. The techniques to choose a single optimal solution from the set of noninferior solutions are also discussed. The impact of multiple decision makers on the selection of a single optimal solution is also described. For illustrative purpose, the two objective model for groundwater management is formulated for potential application related to agricultural use. However, the methodology presented here is equally applicable to a variety of other regional groundwater management problems.

8.1 MULTIOBJECTIVE OPTIMIZATION

Multiobjective Optimization Problem (MOOP) consists of explicitly stated conflicting objectives, and physical, managerial, environmental, social, political and economic constraints as applicable to the planning problem. It determines the optimum value of a vector valued objective function subjected to specified system constraints. The optimal solutions of multiobjective programming models are referred to as the noninferior (nondominated, efficient or Pareto-optimal) solution set. The noninferior solution set is a

subset of the feasible region. Mathematically the multiobjective optimization problem can be expressed as:

$$\text{Maximize} \quad Z(x) = [Z_1(x), Z_2(x), \ldots\ldots, Z_p(x)] \tag{8.1}$$

Subject to

$$g_\varkappa(x) = 0 \quad ; \qquad \varkappa = 1, 2, \ldots, m_1 \tag{8.2}$$

$$h_\varkappa(x) \leq 0 \quad ; \qquad \varkappa = 1, 2, \ldots, m_2 \tag{8.3}$$

$$x \in \Xi \tag{8.4}$$

Where $Z(x)$ is the p-dimensional vector of objective functions; Z_1, Z_2, . ., Z_p are conflicting objectives and x is an n-dimensional vector of decision variables. $g_\varkappa(x)$ and $h_\varkappa(x)$ refer to the equality and inequality constraints respectively. Ξ is the feasible region for the decision variables. The objective functions and the constraints may be either linear or nonlinear.

The most commonly used multiobjective programming techniques to identify the noninferior solutions are the Weighting Method (WM) and Constraint Method (CM). The details of various multiobjective programming techniques are available in Geoffrion (1967), Benayoun et al. (1971), Monarchi et al. (1973), Cohon and Marks (1975), Goicoechea et al. (1982), and Chankong and Haimes (1983).

The constraint method is illustrated here to show how the

developed integrated management models as discussed in previous sections can be easily extended to incorporate the multiple objectives encountered in the planning and management problem. The selection of a particular method for multiobjective optimization depends upon the type of the objective functions. In some situations, weighting method may be computationally more attractive. In order to solve the two objective problem described in section 8.2.1 with minimum modifications of the single objective model algorithm, the constraint method is adopted.

In the constraint method, the MOOP is converted into Single Objective Optimization Problem (SOOP) by treating all the objectives except one as inequality constraints for each solution of the model. The resulting single objective optimization problem can be expresses as:

$$\text{Maximize} \quad Z(x) = Z_1(x) \tag{8.5}$$

Subject to

$$g_\varkappa(x) = 0 \quad ; \qquad \varkappa = 1, 2, \ldots, m_1 \tag{8.6}$$

$$h_\varkappa(x) \leq 0 \quad ; \qquad \varkappa = 1, 2, \ldots, m_2 \tag{8.7}$$

$$Z_\varkappa(x) \geq L_\varkappa \quad ; \qquad \varkappa = 2, 3, \ldots, p \tag{8.8}$$

$$x \in \Xi \tag{8.9}$$

where $L_{\varkappa}$ is the lower bound on the $\varkappa^{th}$ objective. Sequential variations of $L_{\varkappa}$ generate the set of noninferior solutions for the multiobjective optimization problem.

8.2 MULTIPLE OBJECTIVE INTEGRATED MANAGEMENT FOR AGRICULTURAL USE

Agricultural use of groundwater includes irrigation of crops and consumption by livestock. Dependence of agriculture on groundwater resources is common particularly in those areas where surface water is either nonexistent, inadequate or extremely costly to develop. Groundwater withdrawal activities are increasing due to conjunctive use of surface water and groundwater for the optimum utilization of available water resources. In a conjunctive use scenario, groundwater can also provide supplemental irrigation for sibling plantation at the right time or for proper ripening of crops when there is scanty rainfall, and importing small quantities of surface water is not economical. In all these cases, the suitability of the groundwater for agricultural application in a particular agroclimatic region depends on the compatibility between the quality of available groundwater and the quality requirement of existing crops.

Irrigation with groundwater of poor quality or brackish water may cause salinity, specific ion toxicity, or, adversely affect drainage through pores in soils. Excessive salinity may harm the plant growth by reducing the uptake of water through osmotic processes or causing changes in soil structure, permeability and

aeration. Occurrence of these phenomena adversely affect crop production. Different crops have different salt tolerances. The reduction of a particular crop yield due to salinity in irrigation water depends upon its salt tolerance at various stages of the plant growth. Germination and seedling stages are most sensitive to saline irrigation water and any failure in these stages will consequently lead to a reduction in crop production (Hamdy, 1990).

However, use of brackish groundwater and conjunctive use of fresh and saline water have become common irrigation practices for crop production in arid and semi-arid regions. Many researchers have investigated the effects of different irrigation practices and management options on the crop yield when saline water is used for irrigation (Hamdy et al., 1993; Hoorn et al., 1993; Minhas and Gupta, 1993a; Minhas and Gupta, 1993b; Naresh et al., 1993). The suitability of groundwater for irrigation is contingent on the effects of the mineral constituents of water on both the plant and the soil (Richards, 1954; Wilcox, 1955).

Agriculture is of prime economic importance to many nations as a means of producing a significant part of the annual food and fibre needs. Therefore, the water quality problems associated with crop production are of special concern. Therefore, efficient management policies are necessary to increase crop production. Detailed analysis of the trend of salinity sensitiveness to crop yield determines the groundwater quality standards for irrigation application.

An efficient management for higher crop production may need requisite amount (Kumar and Vedula, 1992) of withdrawal of groundwater to irrigate the culturable and cultivated lands. It is also required to meet the desired quality standards depending upon the crop tolerances to different chemical constituents in different locations, and also depending on the trend of reduction in crop production due to irrigation with groundwater of low quality.

The spatial and temporal distribution of groundwater quality in an aquifer can be controlled by adopting a suitable pumping strategy. The required distribution of groundwater quality will depend on the cropping pattern (Lakshminarayana and Rajagopalan, 1977) in the region and therefore, the tolerances of these crops to different chemical constituents in the irrigation water. It is also possible to adopt a conjunctive use strategy where groundwater of poor quality may be mixed with surface water of better quality to achieve a desired quality standard. In these cases the required distribution of groundwater quality will be different and will determine the required pumping strategy to be adopted. Development of an optimal pumping strategy on a regional scale to control groundwater quality can be formulated and solved as a multiobjective optimization problem. A multiobjective optimization problem is characterized by conflicting objectives subject to different physical, managerial and economic constraints.

Evaluation of the optimal policies, and the system tradeoffs obtained as solutions to the problem help in devising a suitable

strategy for the longterm management of water resources in a particular region. These results also help in the assessment and appraisal of the suitability of groundwater resources for agricultural purpose.

A multiobjective management model is formulated for a regional groundwater system to provide an optimal management strategy to control pollution distribution in the aquifer as per agricultural needs and to evolve an optimal allocation policy to satisfy irrigation demands. The model is based on the nonlinear optimization model which describes the flow and transport processes occurring within the groundwater system and the considered objectives and constraints. The model evaluates the pumping schedule in terms of spatial pattern to make the aquifer usable for irrigation of different crops in different agroclimatic regions. A Pareto-optimal solution of the two system objectives is established. The present study considers two different conflicting objectives: (i) minimization of total withdrawal from the entire region over a specified time horizon, and (ii) minimization of the maximum allowable concentration of a conservative pollutant occurring in the groundwater. Other implicit objectives that are considered as constraints are the distribution of resulting hydraulic heads in the aquifer. The hydraulic heads obtained as a result of implementing the optimal management decisions are also analyzed. The spatial distributions of chloride concentration in different management periods determine whether the available groundwater can be used for

various crops. These results as obtained from this model, or, a slightly modified model, will be helpful in establishing different optimal irrigation strategies when conjunctive use of saline water and fresh water from other sources is possible.

8.2.1 Management model

A bicriterion programming model is formulated for groundwater pollution management to meet the agricultural demands of desired quality. The explicit conflicting objectives considered are: (i) minimization of total withdrawal from the entire region over a specified time horizon and (ii) minimization of the maximum allowable concentration of a conservative pollutant occurring in the groundwater. Mathematically these objectives can be expressed as:

$$\text{Minimize} \quad Z_1 = \sum_{k=1}^{nts} \sum_{i,j \in I} (Q_p)_{i,j}^{k} \tag{8.10}$$

$$\text{Minimize} \quad Z_2 = \left[\text{Maximum}\left(C_{i,j}^{k}\right)\right]; \quad i,j \in I,\ k = 1,\ nts \tag{8.11}$$

Where, I denotes a set of specified grid locations (i,j). nts is the number of time steps considered within a planning horizon.

The system constraints are the simulation constraints which govern the flow and transport processes occurring within the groundwater system, and the physical, managerial and other constraints if any. The simulation constraints are based on the

groundwater flow and solute transport equations as described in Chapter 3. Thus, simulation constraints are expressed as:

$$(g_f)^k_{i,j} = 0 \tag{8.12}$$

$$(g_t)^k_{i,j} = 0 \tag{8.13}$$

The lower and upper bounds on the decision variables are:

$$(h_{lb})^k_{i,j} \leq h^k_{i,j} \leq (h_{ub})^k_{i,j} \tag{8.14}$$

$$(Q_{lb})^k_{i,j} \leq (Q_p)^k_{i,j} \leq (Q_{ub})^k_{i,j} \tag{8.15}$$

$$(C_{lb})^k_{i,j} \leq C^k_{i,j} \leq (C_{ub})^k_{i,j} \tag{8.16}$$

Where, $i, j \in I$; $k = 1, nts$.

The lower bounds on hydraulic heads are chosen such that the aquifer does not become unconfined. The upper bounds on hydraulic heads are chosen such that the area does not become waterlogged. These bounds may be modified also as per imposed political or managerial requirements if appropriate.

The lower bounds on pumping variables are estimated based on the water required for irrigation from groundwater sources, depending upon the water requirement for a crop in a particular agroclimatic region, and the irrigation practice to be adopted. The

upper bounds on pumping variables are estimated based on the pumping capacity of the pump to be installed. The procedure of estimating these bounds is discussed in Chapter 3. If the objective is only to control the pollution during the planning period such that the spatial distribution of pollutant satisfy the desired quality standard for a crop, the lower bound on pumping becomes simply nonnegative.

Since the quality of groundwater is considered as an explicit objective to obtain the noninferior solution set, the upper bounds on concentration variables become redundant. The lower bounds on concentrations will be generally specified as nonnegative only.

8.2.2 Method of solution

The two-objective optimization model as stated above is transformed into a single objective optimization model using the constraint method. The resulting model can be expressed as:

$$\text{Minimize} \quad Z_1 \tag{8.17}$$

Subject to

$$(g_f)^k_{i,j} = 0 \quad ; \quad i,j \in I,\ k = 1,\ nts \tag{8.18}$$

$$(g_t)^k_{i,j} = 0 \quad ; \quad i,j \in I,\ k = 1,\ nts \tag{8.19}$$

$$Z_2 \leq U \tag{8.20}$$

$$x \in \Xi \qquad (8.21)$$

The functions $(g_f)^k_{i,j}$ and $(g_t)^k_{i,j}$ represent the equality constraints defined by left hand side terms of Equations (3.46) and (3.88) respectively. U is the upper bound on the second objective. The sequential variation of U generates the set of noninferior solutions for the considered biobjective optimization model. The bounds on the decision variables remain the same as described by inequalities (8.14) to (8.16).

The embedding technique is used to incorporate the simulation constraints into the optimization model. The resulting single objective optimization model is a constrained nonlinear optimization model. This is solved using Exterior Penalty Function Method (EPFM) in conjunction with Hooke-Jeeves (HJ) algorithm of pattern search method. The descriptions of these methods are discussed in Chapters 3 and 4.

The optimization procedure requires the specification of certain optimization parameters. These parameters are r, α_h, α_q, α_c, β_h, β_q, β_c, ε_h, ε_q and ε_c. r is a set of penalty parameters. α, β and ε denote respectively reduction factor, acceleration factor and termination parameter. The suffix h, q and c denote the class of hydraulic head, pumping and concentration variables respectively. These optimization parameters are discussed in Chapters 3 and 4.

8.2.3 Sequential variation of U

An exhaustive set of noninferior solutions is infinite. In order to generate a finite number of noninferior solutions, some guidelines are necessary to fix the range of interest for U. Optimal solutions of the transformed single objective optimization model are obtained for different values of U within the range of interest. The range of interest is estimated based on the desired water quality standard for irrigation, irrigation practice, and probable reduction in crop yield due to use of poor quality of water. Table 8.1 gives general guidelines for salinity and chloride limits in irrigation water (Roscoe Moss Company, 1990). Table 8.2 gives some guidelines for the reduction of crop yield in Indian saline areas due to the use of different qualities of saline water for irrigation.

8.2.4 Results and discussions

Fig. 8.1 shows a finite difference network for the study area of 900 ha (3 km x 3 km) divided into square cells, each of size 0.5 km x 0.5 km with Dirichlet boundary condition. The aquifer is assumed homogeneous and anisotropic. The hydraulic conductivities, K_{xx} and K_{yy} are 5.0×10^{-4} m/s and 4.0×10^{-4} m/s respectively. The storage coefficient, effective porosity, thickness of leaky layer, saturated thickness of confined aquifer, hydraulic head in source bed and ground surface elevation are respectively 2.0×10^{-4}, 0.3, 2.0 m, 30.0 m, 55.0 m, and 62.0 m. These values do not change with respect to space and time. The vertical hydraulic conductivity of

Table 8.1 Salinity and chloride limits in irrigation water

Quality of irrigation water	Unit	Degree of Restriction on Use		
		None	Slight to Moderate	Severe
Salinity				
EC	µmho/cm	< 700	< 700 - 3000	> 3000
TDS	mg/l	< 450	< 450 - 2000	> 2000
Chloride				
Surface irrigation	meq/l	< 4	< 4 - 10	> 10
	mg/l	< 140	< 140 - 350	> 350
Sprinkler irrigation	meq/l	< 3	> 3	
	mg/l	< 100	> 100	

Source: Roscoe Moss Company (1990)

Table 8.2 Reduction of crop yield in Indian saline area

Reduction in crop yield (location: Agra)	Salinity limits (dS/m) for Wheat	for Rice	Sorghum
90%	6.6	2.3	7.0
75%	10.4	4.6	11.2
50%	16.8	8.6	18.1

Source: Gupta et al. (1994)

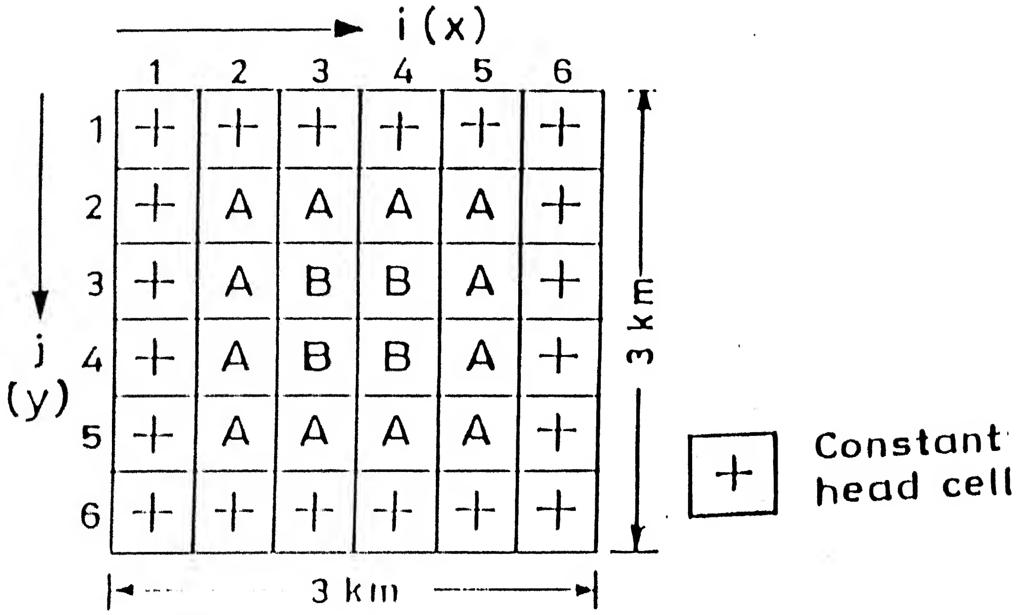

Fig. 8.1. Finite difference network.

overlying leaky layer is 1.0×10^{-10} m/s when leakage is considered. The vertical point recharge in all the cells except boundary cells, when applicable is assumed 1.0 l/s throughout the management period. The recharge at all boundary cells is assumed zero. The solute considered here is chloride, a conservative pollutant. The concentration of chloride entering the internal cells denoted by A and B are respectively 100 mg/l and 200 mg/l in recharge, and 100 mg/l and 150 mg/l in leakage. The longitudinal and transverse dispersivities are 30 m and 10 m respectively. Two time steps are considered for a time horizon of one year. The solution can be easily extended to longer time horizons and larger number of time steps as required.

In the top layer of boundary cells (Fig. 8.1), the hydraulic heads are specified as 50.0 m. In the bottom layer of boundary cells, the hydraulic heads are specified as 41.0 m. For the remaining cells, simple interpolation is used to obtain the head distribution, which are the specified initial heads. Existing concentrations at all boundary cells are specified as 100 mg/l. The initial concentration in the aquifer for the cells denoted by A and B (Fig. 8.1) are 200 mg/l and 400 mg/l respectively.

The optimization parameters used for the computation are $r = 10^{-18}$, $\alpha_h = \alpha_q = \alpha_c = 2$ and $\beta_h = \beta_q = \beta_c = 1$. Optimization runs are started with initial values of 40.0 m, 50 l/s and 100.0 mg/l for hydraulic head, pumping and concentration variables respectively. The values for ε_h, ε_q and ε_c are taken 0.001 m, 0.01 l/s and 0.01

mg/l respectively. The starting step sizes are assumed 0.5 m for hydraulic head, 5 l/s for pumping and 10 mg/l for concentration variables. All computations have been performed on a HP 9000/735 computer system having a performance of 40 MFLOPS.

Fig. 8.2 shows the Pareto-optimal solutions of the objectives under consideration. It shows that if better quality of groundwater is desired, the required pumping will be more. Thus, the resulting cost of pumping will be more. Although crop yield will be more if groundwater of less salinity is used, the cost of water to be used for irrigation also increases. The best compromise solution can be achieved by applying either the Surrogate-Worth Tradeoff (SWT) method (Chankong and Haimes, 1983) or the utility function approach.

To determine a single optimal solution for the multiobjective problem, it is required to obtain the preference ordering of the Decision Makers (DMs) regarding the objectives under consideration. These preference orderings are based on the explicit or implicit utility functions of the DMs. In this particular problem, these preference orderings will depend upon the quality of water that will be available for irrigation and the resulting net benefits from the crop yield.

The leakage and recharge occurring in the aquifer dilute the chloride concentration and hence, the amount of pumping required to attain the desired quality distribution decreases. However, as shown in Fig. 8.2, this decrease in required pumping is marginal. The role of leakage and recharge will become significant as the vertical

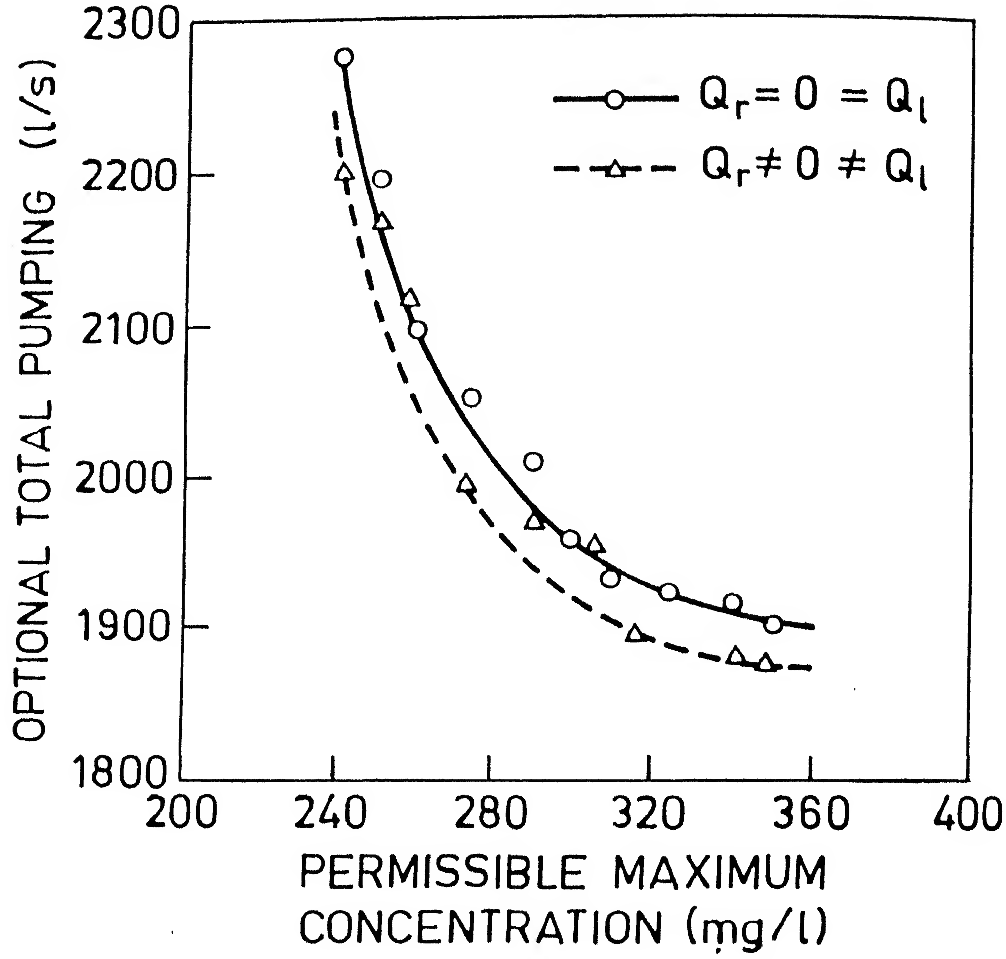

Fig. 8.2 Pareto-optimal solutions for the two-objective model.

conductivity of the leaky layer increases and/or the quality of recharge and leakage improves.

Figs. 8.3 and 8.4 show the spatial distribution of optimal pumping in the first and second management periods (each of 6 months duration) respectively if the maximum permissible concentration (U) in the study area is limited to 350 mg/l. These results correspond to the confined aquifer having no point recharge. The pumping required in the first management period (960.70 l/s) is more than that in the second management period (941.58 l/s). It occurs because, after first management period, better quality distribution results due to removal of chloride from the aquifer by pumping in the first management period, and also due to increased recharge of better quality water from the boundary cells.

The spatial distributions of chloride concentration in the aquifer after implementing the management decisions regarding the optimal pumping are shown in Figs. 8.5 and 8.6. These distributions provide the guidelines for deciding the cropping pattern and irrigation practice to be adopted. Molecular diffusion has been neglected because of its negligible contribution in the computation of the distribution of chloride. It is evident from the fact that at optimal condition, Peclet number varies between 2.00 and 11.40. At initial condition, Peclet number varies between 2.00 and 2.67. Therefore, the change in chloride distribution with space and time is occurring mainly due to advection, mechanical dispersion, pumping and recharge of better quality of water from the boundary cells.

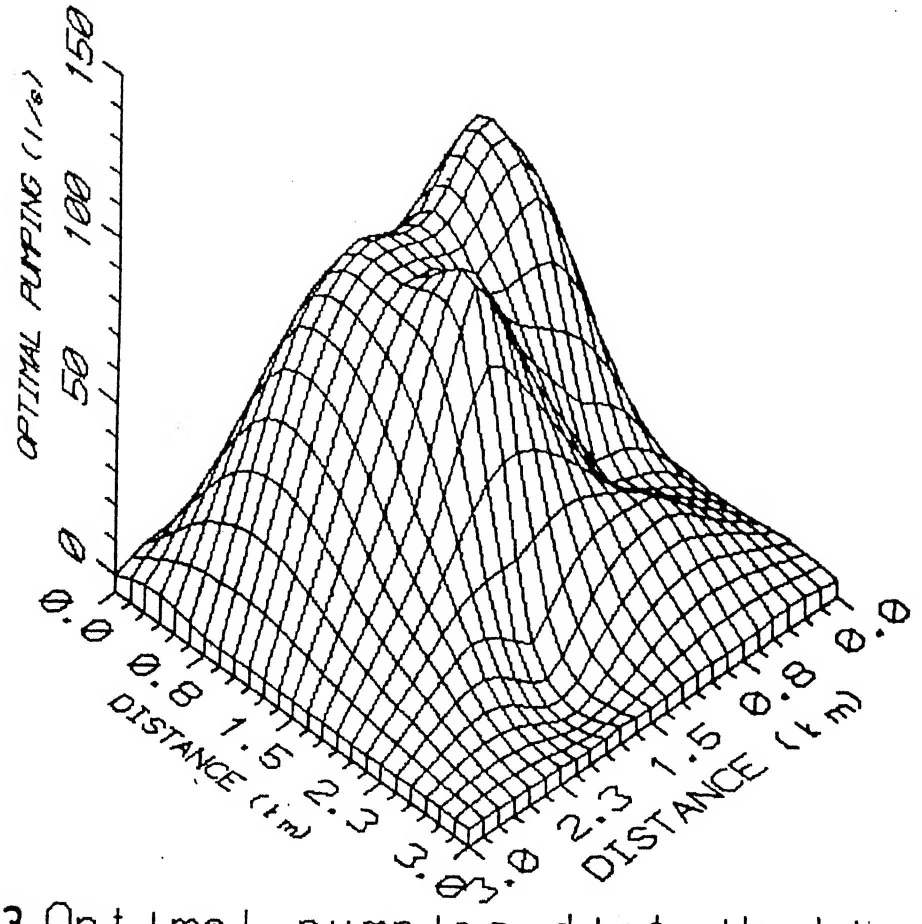

Fig. 8.3 Optimal pumping distribution in first management period

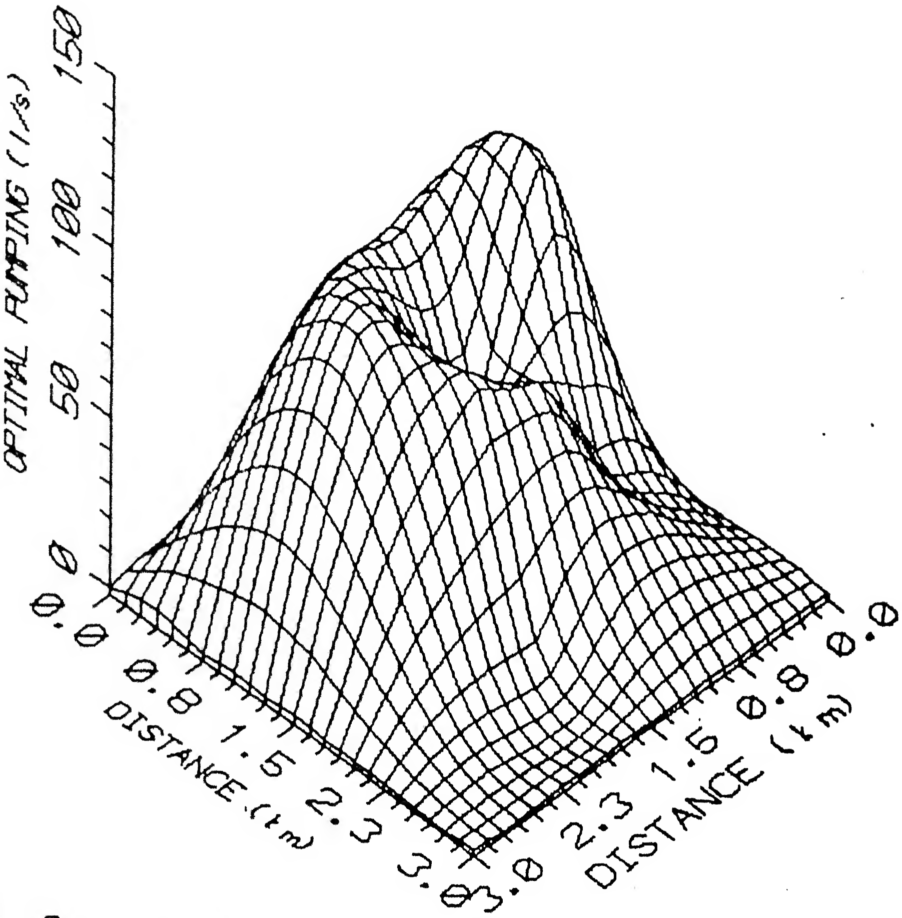

Fig. 8.4 Optimal pumping distribution in second management period

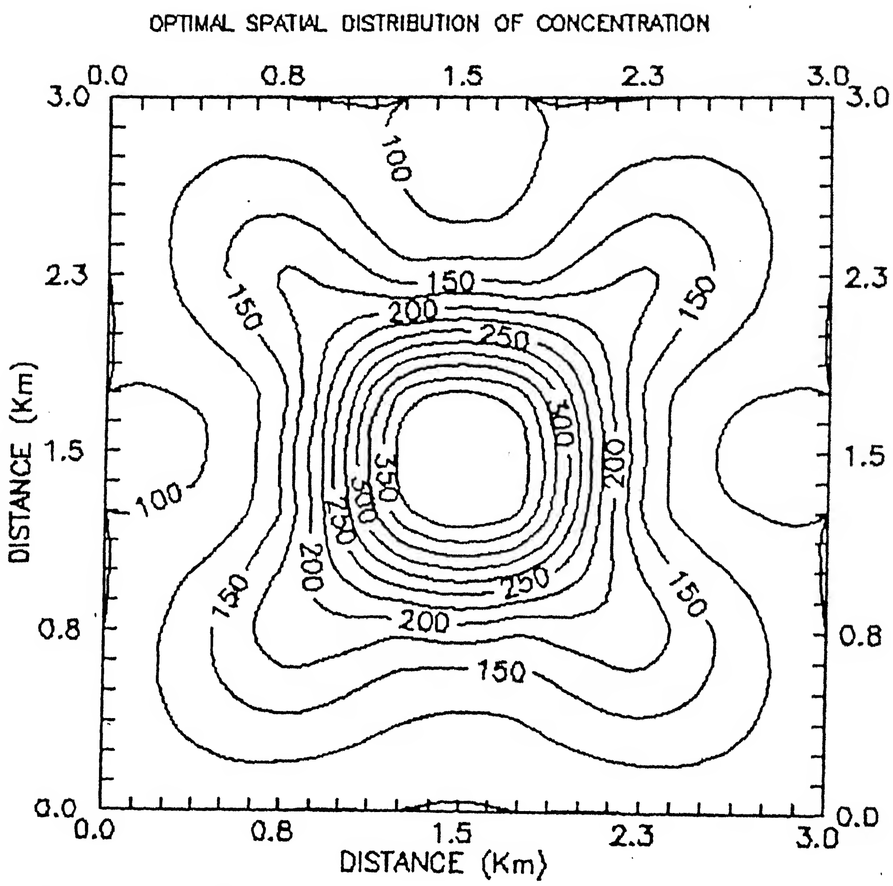

Fig. 8.5 Chloride concentration (mg/l) distribution at the end of first management period

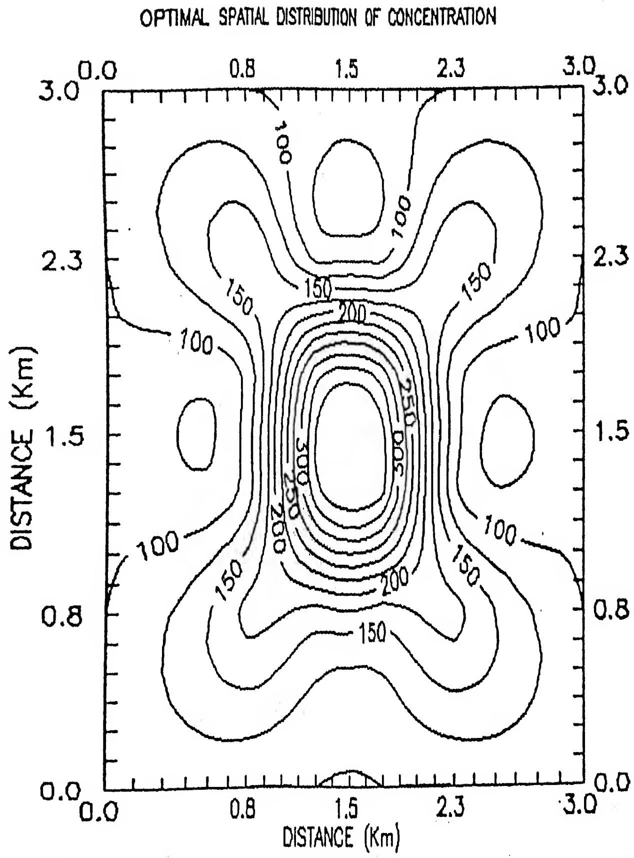

Fig. 8.6 Chloride concentration (mg/l) distribution at the end of second management period

The distribution of hydraulic heads after optimal pumping in first and second management periods are shown in Figs. 8.7 and 8.8 respectively. The change in hydraulic head distribution occurs due to pumping and natural recharge from the boundary cells. These distributions will help in the management of groundwater resource for agricultural applications in subsequent crop seasons. It determines the availability of groundwater for irrigation purpose in quantifiable units.

If it is desired to allow the maximum permissible chloride concentration of 250 mg/l throughout the area under consideration by the end of one year period, the required optimal pumping schedule from the aquifer to achieve this target is tabulated in Table 8.3. After implementing this management decision, the hydraulic head distribution after one year is shown in Fig. 8.9. The impact of quality constraints on hydraulic head distribution is evident from Figs. 8.8 and 8.9. Thus, the quality requirement also determines the potential for groundwater use. The resulting spatial distribution of chloride concentration due to implementation of this optimal management policy is shown in Fig. 8.10. The results reported in Table 8.3 reveal that the most appropriate locations of wells for pumping to restore the aquifer within the desired quality are (2,2), (3,2), (3,3), (3,4), (4,2), (4,3), (4,4), and (5,2). Other eight cells are relatively ineffective for this purpose. It implies that there is no need of having pumping wells in these ineffective cells. Therefore, the optimal allocation of wells and its optimal pumping

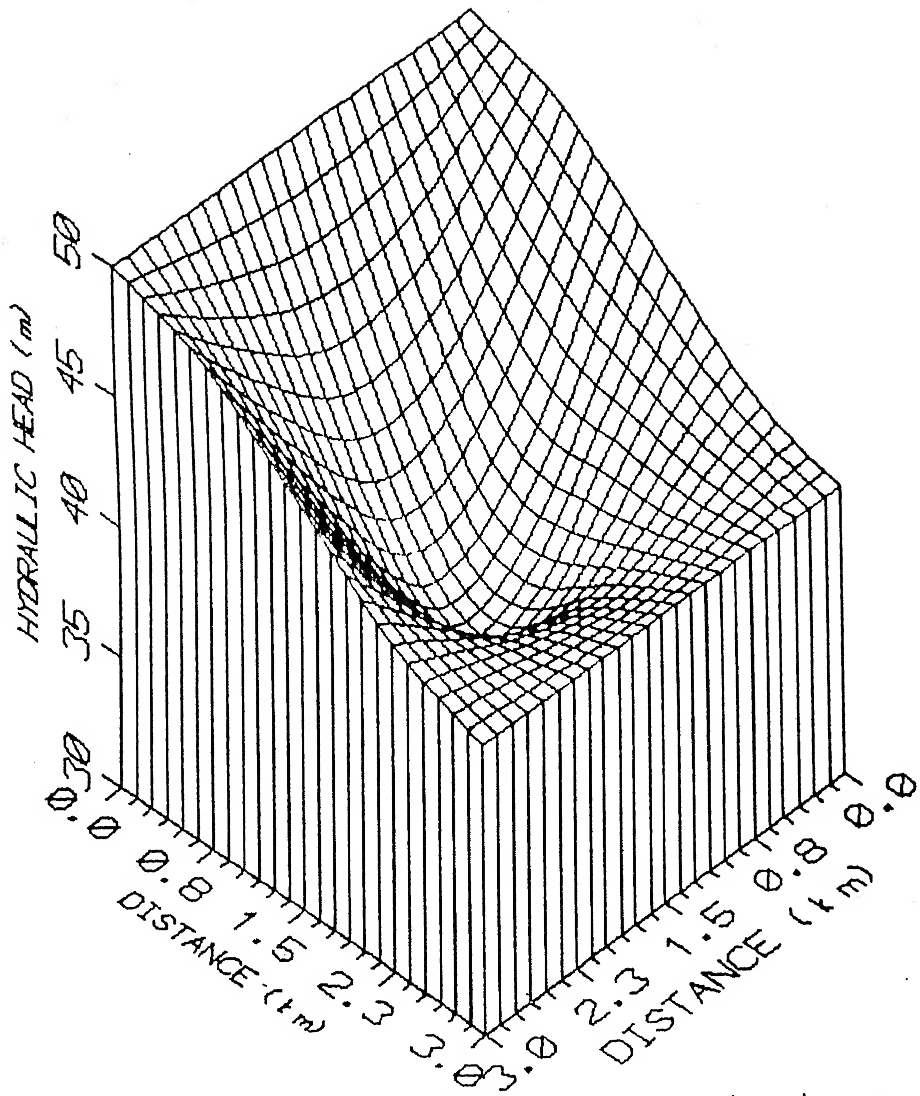

Fig. 8.7 Hydraulic head distribution at the end of first management period

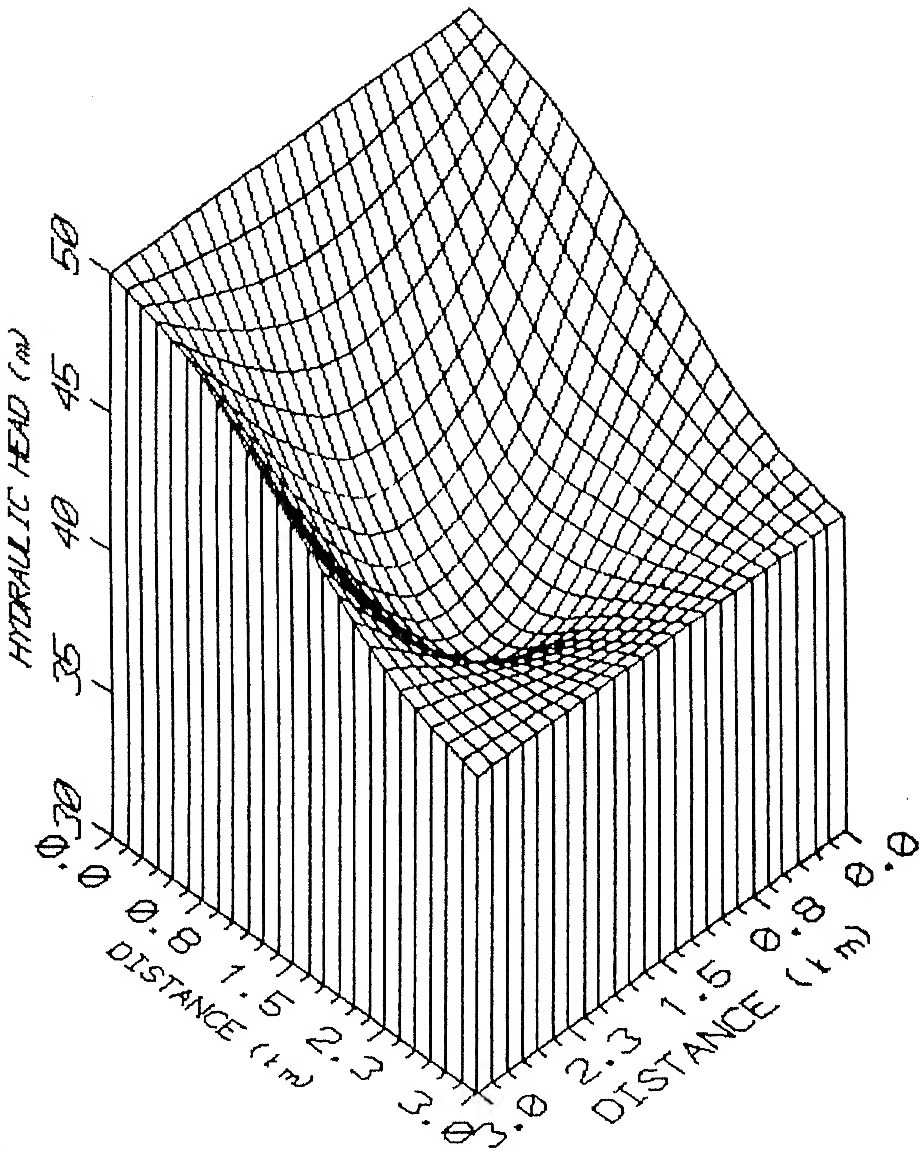

Fig. 8.8 Hydraulic head distribution at the end of second management period

Table 8.3 Spatial optimal pumping schedule

Cell location		Optimal pumping (l/s) in management period	
i	j	1	2
2	2	97.9200	49.8630
2	3	0.0098	0.0098
2	4	0.0098	0.0098
2	5	0.0098	0.0098
3	2	45.8200	56.0740
3	3	214.4000	146.6800
3	4	225.6700	239.2600
3	5	0.0000	0.0000
4	2	49.7070	30.0680
4	3	234.7200	190.8800
4	4	224.9300	253.9200
4	5	0.0098	0.0098
5	2	44.7560	85.1950
5	3	0.0098	4.5898
5	4	0.0098	0.0098
5	5	0.0098	0.0098

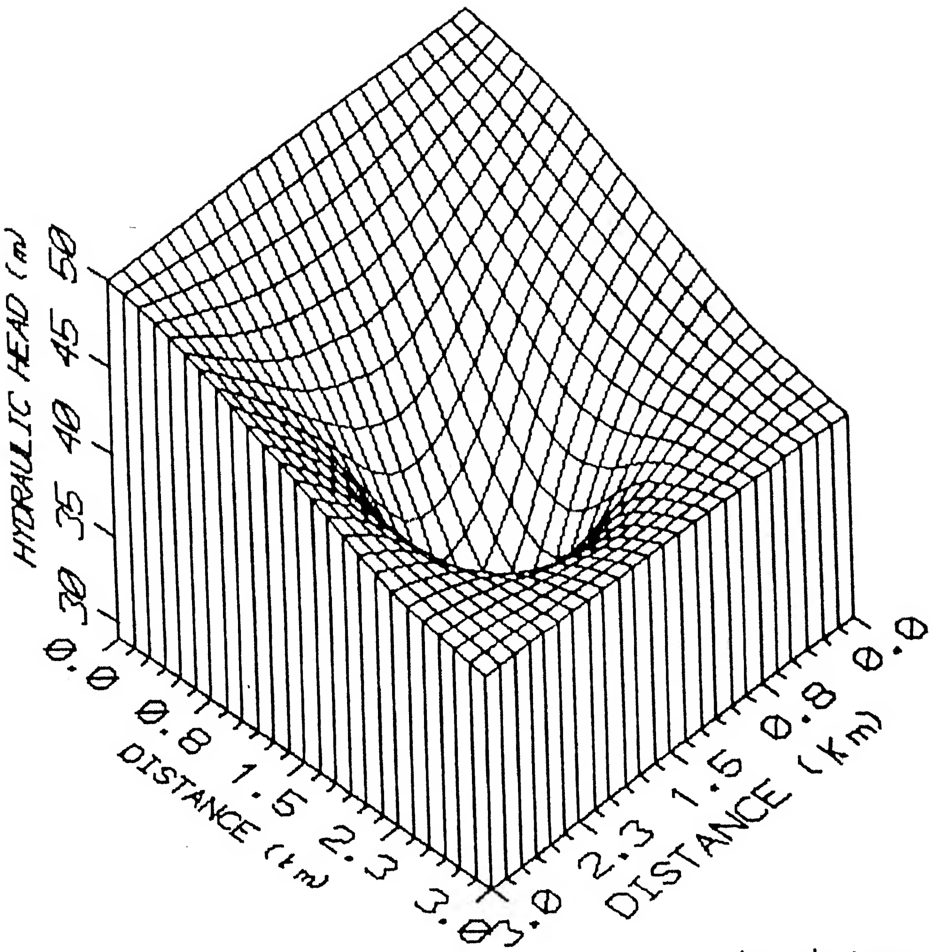

Fig. 8.9 Hydraulic head distribution after one year

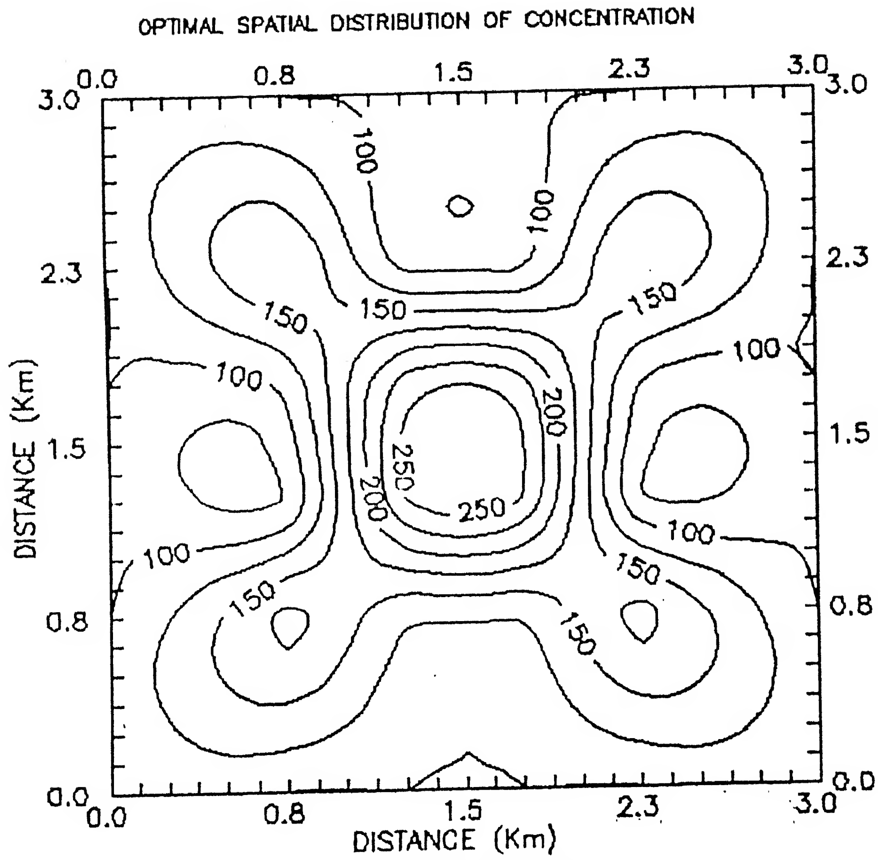

Fig. 8.10 Chloride concentration (mg/l) distribution after one year

rates make the management policy more cost effective. The optimal well locations are shown in Fig. 8.11.

It should be noted that obtained solutions may be a local optimum or a global optimum. To ensure the global optimality of the solution, an exhaustive search of all local optimal solutions are necessary. This is an inherent limitation of most constrained nonlinear optimization algorithms.

8.3 CHOOSING A SINGLE OPTIMUM SOLUTION FROM NONINFERIOR SOLUTIONS

Solution of a multiobjective optimization problem using constraint method yields a set of noninferior solutions. However, only one single solution can be implemented. The best compromise solution to be adopted from these noninferior solutions can be identified only when the preference ordering of the decision maker is available explicitly or obtained sequentially. These preference orderings are based on the explicit or implicit utility functions of the decision maker (DM) with respect to the multiple objectives being considered. Often it is very difficult to obtain an explicit utility function of the DM. Therefore, a more practical approach is to order the noninferior solutions based on the implicit utility functions. The surrogate worth tradeoff method (Chankong and Haimes, 1983) is based on the derivation of the implicit utility function of the DM to identify the best compromise solution.

The surrogate worth tradeoff method was originally developed by Haimes and Hall (1974). It consists of four steps: (1) generate a

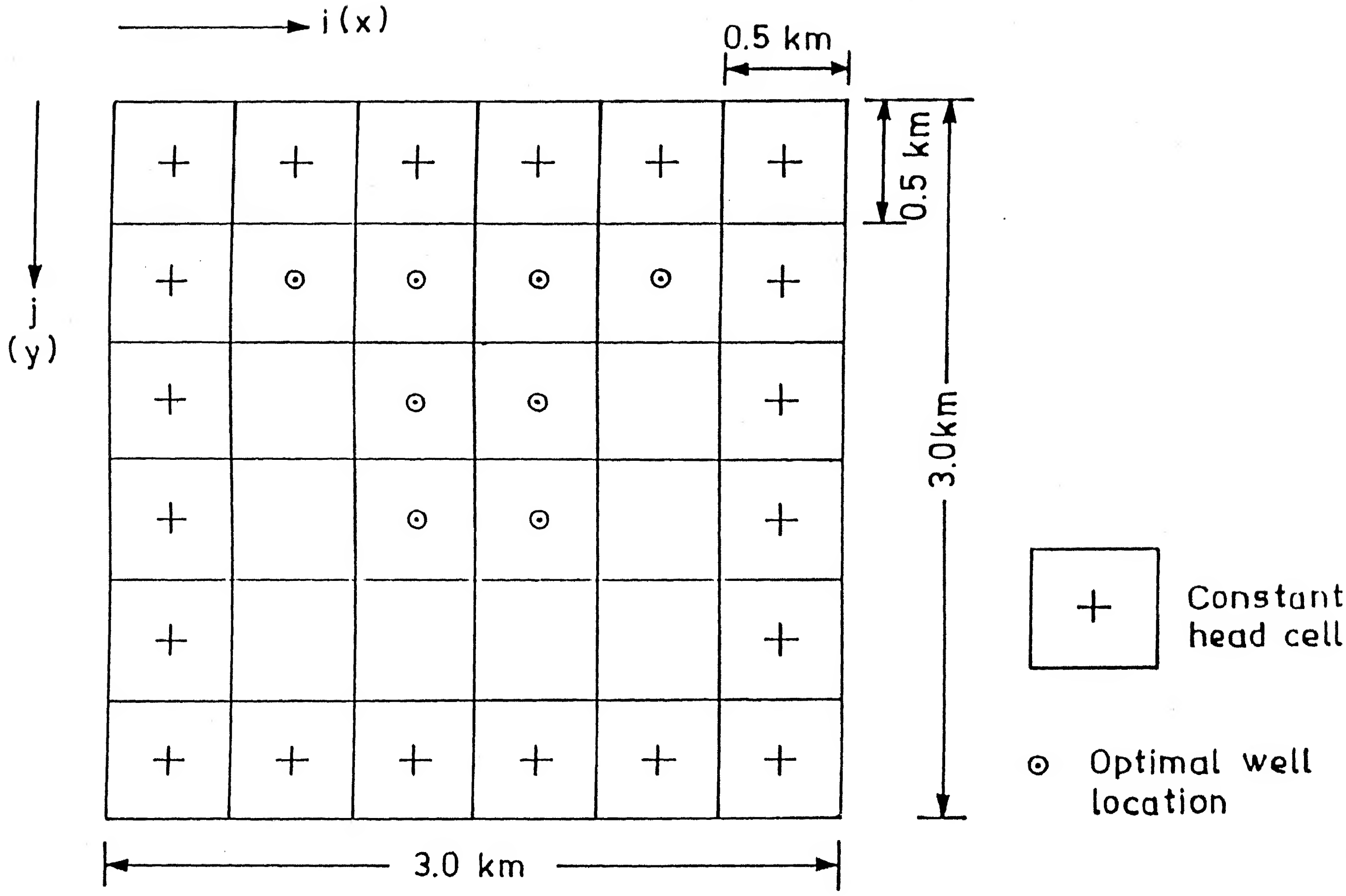

Fig. 8.11. Optimal well locations to maintain 250 mg/l chloride concentration by the end of one year period.

resources involving public welfare are made collectively by a group of members and decision makers. Such type of situations frequently arise in the planning and management of water resources systems. The decision making group may comprise of members of the board of directors of a large corporation, experts from academic or research institutions, and professionals working in the field, elected representatives in a legislative body or other public representatives in a political system. For example, a decision group for planning and management of a large scale groundwater system will consist of scientists and engineers from water, agriculture and geology fields, environmentalists, economists, even top government officials and representative persons from the areas being affected or benefited by this plan. Thus, the final decision regarding the managerial problem rests with multiple decision makers.

The multiple decision makers may have conflicting opinions, because each decision maker in the group will have own characteristic interpretation of the significance and relative values of the objectives under consideration. In addition, if a decision maker is a representative of another group of individuals, he may well be responsive to the views of his constituency. Sometimes, the people of the area where the management problem is going to be implemented, may have adverse assessment of the significance of a particular objective, and hence influence the relative weights assigned to the objectives by the decision makers.

It is clear from the above discussion that most planning and

management problems of public interest such as the groundwater management problems involve a number of decision makers. The relative weights assigned to different objectives under consideration are a subjective decision based on different opinions of involved decision makers, in addition to the technical assessment and appraisal of the solutions. The SWT method extended for multiple decision makers is one possible means to resolve conflicting priorities of multiple decision makers, using the indifference band approach. However, an universally acceptable solution to this problem still eludes us.

8.5 SUMMARY

A multiobjective constrained nonlinear optimization model is formulated and solved for evolving optimal groundwater withdrawal strategy for agricultural use in a given area. The two conflicting objectives considered are: (i) minimization of pumping requirements, and (ii) minimizing the maximum concentration of a pollutant in the aquifer. Physical constraints representing the flow and transport processes, boundary conditions and other required managerial constraints are also imposed.

The main advantage of using the formulated model is the interlinking of the simulation model required to simulate the flow and transport processes and the optimum decision model. This characteristic of the management model is achieved using the embedding approach. Therefore, the formulated model avoids the

linking of simulation model externally to the optimization model. It also avoids the linearization of involved nonlinear objectives and constraints, due to the application of nonlinear programming algorithms.

The Pareto-optimal solutions obtained as solutions of the two-objective model show the tradeoff between the two noncomensurate objectives. These noncomensurate objectives are pumping requirement (a surrogate for economic cost of pumping) and the maximum concentration of a pollutant that is permitted for agricultural use of the groundwater. These tradeoffs are necessary to establish the feasibility of using the groundwater for different crops and hence, for planning the cropping pattern and irrigation practices in the area. The economic returns from different types of crops together with respective yields, and the required cost of pumping to achieve a specified quality standard will determine the selection of a single optimal point within the set of Pareto-optimal solutions that were generated.

The single optimal solution from the set of noninferior solutions can be selected using information regarding the utility function of the decision maker. A simplified approach to achieve the same is the surrogate worth tradeoff method. However, the selection of a single optimal solution is affected if multiple decision makers are involved in the decision process.

The spatial and temporal distribution of pollutant concentration and hydraulic heads in the aquifer obtained as

solutions of the management model ensure the usability of the groundwater resources for agricultural purpose in subsequent crop seasons. The formulated model is equally adoptable for various agroclimatic regions and cropping patterns.

Conjunctive use of surface water and groundwater is not explicitly considered in this model. However, minor modifications in the constraints and the first objective function can accommodate conjunctive management strategies. Other relevant issues like uncertainties in parameter estimations, accuracy of specifying boundary conditions, and finally the limitations of nonlinear optimization algorithms in locating a global optimal solution are no doubt other important issues that should be considered in actual planning and management.

SUMMARY, CONCLUSION AND SCOPE FOR FUTURE WORK

CHAPTER 9

SUMMARY, CONCLUSION AND SCOPE FOR FUTURE WORK

9.1 SUMMARY

Groundwater constitutes an important component of many water resources systems that are traditionally developed as sources of municipal, industrial, agricultural and horticultural water supply. Planned withdrawal of groundwater is important particularly in those areas where surface water is nonexistent, inadequate, extremely costly to develop, or surface water of desired quality is not available. Now a days, deteriorating quality of groundwater is causing more concern to both suppliers and users of water. This is becoming a serious problem in all industrialized, urbanized and even in rural areas due to various natural and man-made activities, and catastrophic events. Therefore, potential utilization of groundwater not only depends upon the availability of water in desired amount, but more crucially depends upon its quality that should match with

the desired or specified quality for intended use. Due to the significance of the quality aspect, an integrated management which deals with both quality and quantity aspects in a single framework is drawing greater attention for either integrated basin scale development, regional scale development, larger scale development, smaller scale development, or even for an individual well projects.

In recent years, many simulation and management models have been developed to analyze the steady and transient groundwater pollution problems. However, majority of the management models used the simplifying assumptions of linear systems and restricted the models to linear objective functions and constraints. Comparatively less attention has been provided on accurate and adequate modeling of the nonlinearities especially inherent in the solute transport process. Nonlinear objective functions and constraints were less frequently used. However, many realistic problems may require modeling the inherent nonlinearities, while incorporating nonlinear managerial or other constraints and objectives. No large scale application of the embedded technique has been reported for the transient pollutant management models. Some management models are not even fully embedded. Some generic aspects of modeling such as uncertainties and risks involved in the modeling have been scarcely addressed. The present study is devoted mainly to the formulation and development of an integrated groundwater management model for regional groundwater management using embedding technique; and to the development of the methodologies for its solution using

nonlinear programming techniques under different physical, managerial and operational situations.

An integrated groundwater management model is formulated as a constrained nonlinear optimization problem. The quality and quantity aspects of the groundwater system are conflated in the developed model. To simulate the physical and chemical processes occurring within a leaky confined aquifer system, the coupled set of flow and pollutant transport equations are incorporated into the management model using Embedding Technique (ET). The blended use of quality and quantity aspects into the optimization model avoids the necessity of linking an external simulation model with the optimization model. Thus, the flow and transport processes are simulated within the model. In addition, this model is capable of incorporating other imposed managerial and physical constraints so that the developed optimal policies are operationally, socially, environmentally, economically, financially and politically feasible. This management model is solved using Nonlinear Programming (NLP) because, the embedded solute transport equations are nonlinear. The developed methodology can be used to solve optimization models containing nonlinear constraints and/or nonlinear objectives. Application of NLP also eliminates the necessity of linearizing nonlinear constraints.

Assuming the aquifer as a distributed parameter system, the two-dimensional flow and solute transport equations are discretized using Finite Difference Method (FDM) in a strong implicit form.

These discretized equations are embedded into the optimization model as simulation constraints. The discretized solute transport equation includes the dispersive, diffusive and degradable components in addition to the advective component. However, for illustrative purpose, the applicability of the developed methodology has been demonstrated for cases in which convective diffusion predominates over molecular diffusion. Three types of boundary conditions namely, Dirichlet type, Neumann type and Cauchy type are considered for illustrating the performance of the model.

The developed multivariable constrained nonlinear optimization models are converted to multivariable unconstrained nonlinear optimization models using the Exterior Penalty Function Method (EPFM). The method is chosen over Interior Penalty Function Method (IPFM) to avoid the necessity of specifying an initial feasible solution. The EPFM is also preferred over the IPFM to eliminate some other computational difficulties especially associated with nonlinear equality constraints. The sequential unconstrained minimizations of the resulting composite objective functions are carried out using two different pattern search methods namely, Hooke-Jeeves (HJ) method and Powell's Conjugate Direction (PCD) method. The PCD method employs the Quadratic interpolation technique (QFIT) for one dimensional search which uses Equal Interval Search Technique (EIST) for bracketing the optimum in one dimensional search. These two methods are preferred over gradient based methods mainly because, evaluations of derivatives are not required and many

other computational difficulties are eliminated.

The applicability and suitability of these two methods (HJ and PCD) are explored in terms of its robustness, versatility, accuracy, efficiency and computational feasibility. The necessary modifications required in the implementation of the HJ and PCD algorithms for solution of various groundwater management problems are devised and incorporated in the methodology presented. Nonlinear test problems are solved using the developed algorithms and then compared with the exact solutions to validate the coded algorithms. The performance of the developed integrated management model is also tested extensively for descriptive evaluation. The effects of time and space discretization, penalty parameter, and initial solution on the optimal solution are discussed. The significance of the estimation of initial penalty parameter value is examined and a strategy is devised to update it for the sequential unconstrained minimization of the objectives involved in the groundwater management problems.

The applicability of the model is illustrated for four distinct types of groundwater management problems. These problems are: (i) Integrated management for groundwater supply, (ii) Integrated management for groundwater remediation, (iii) Radionuclide pollutant management, and (iv) Special case of quantity management. The first and second categories of problems deal with a conservative pollutant, chloride. The third problem deals with a radioactive pollutant, tritium. The fourth problem deals with a groundwater

extraction problem in which either quality aspect is irrelevant or ignored. Basically, all these problems are solved by two models: the first one maximizes the objective function and the second one minimizes the objective function.

The first model (Model I) is applicable for the first, third and fourth problems. Model I aims at finding the optimal pumping policies for maximizing the groundwater withdrawal from the aquifer in a planning horizon subject to imposed physical and managerial constraints. The second model (Model II) which is applicable for the second problem. Model II aims at finding the optimal pumping policies for minimizing the groundwater withdrawal from the aquifer in a planning horizon, to restore the aquifer upto desired quality under specified operational conditions. The problems are solved to assess the significance of adequately modeling the system and to evolve optimal policies for different aquifer environment and operating conditions.

The solutions are obtained for different management scenarios representing different boundary conditions, aquifer parameter estimates, physical and managerial constraints, and natural and man-made processes affecting the groundwater system. Some generic aspects of modeling such as uncertainties associated with aquifer parameters are illustrated through the deterministic and randomized modeling of hydraulic conductivity. The optimal solutions for groundwater remediation problem are obtained for different planning periods and operational conditions. The effect of variability of

specified potential pumping locations on the optimal solution is also examined. Issues related to the cost of installation of new wells and undesirable consequences of implementing a management policy are addressed in the context of selection of an optimal management strategy.

A comparative study of HJ and PCD methods is carried out to assess the applicability and suitability of these two methods for the solution of various groundwater management problems. These comparisons are made in terms of accuracy, efficiency, robustness, ease in implementation and computational feasibility. Solutions for different management scenarios are obtained using both the methods in conjunction with exterior penalty function method and these solutions are then compared. In addition, the computational difficulties encountered during the development of the methodologies and the remedial measures adopted are discussed with proper explanation.

The proposed integrated management model (Model II) is extended to a multiobjective management model in order to evolve policies when conflicting objectives are involved. The formulation, development and solution of the multiobjective management model with two conflicting objectives are illustrated. Solutions of this model provide an optimal management strategy to control pollution distribution in the aquifer as per agricultural needs and at the same time evolve an optimal allocation policy to satisfy irrigation demands. Pareto-optimal solutions representing the tradeoff between

the two noncomensurate objectives are obtained using the Constraint Method (CM). The two conflicting objectives considered are: (i) minimization of pumping requirements, and (ii) minimizing the maximum concentration of a pollutant in the aquifer. Physical constraints representing the flow and transport processes, boundary conditions and other required physical, managerial and operational constraints are also imposed. Tradeoffs are established to study the feasibility of groundwater use for different cropping patterns and irrigation practices in different agroclimatic conditions in a particular area. The spatial and temporal distributions of pollutant concentration and hydraulic head are examined to ensure the usability of groundwater resource for agricultural purpose in subsequent crop seasons. The impact of multiple decision makers on the selection of a single optimum solution from the generated noninferior solutions using surrogate worth tradeoff method or some other utility function approach are also discussed.

9.2 Conclusions

The conclusions specific to various problems studied are not repeated here, only the general conclusions of this study are enumerated below:

1. The developed methodologies can be used for regional scale management of groundwater systems.
2. The embedded optimization model is suitable for optimal management of groundwater pollution and groundwater withdrawal.

The embedding technique eliminates the requirement of linking flow and transport simulation models to the optimization model externally.

3. The blended use of the coupled set of flow and solute transport equations as simulation constraints in the developed integrated management model enables the decision makers to evolve management policies for optimal use of groundwater and its sustainable development in terms of both quantity and quality.
4. The developed methodologies can be used to solve optimization models containing nonlinear constraints and/or nonlinear objectives. Application of NLP also eliminates the necessity of linearizing nonlinear constraints.
5. The Hooke-Jeeves method in conjunction with exterior penalty function method (EPFM & HJ) appears more robust and versatile in its applicability and suitability to solve various groundwater management problems. However, in some situations the Powell conjugate direction method in conjunction with exterior penalty function method (EPFM & PCD) may prove to be more efficient in locating the optimal solution.
6. Rate of convergence of EPFM & PCD is more than EPFM & HJ, but the former requires more CPU time and computer memory storage.
7. The solution results obtained are dependent on specified initial solution, penalty parameter values and optimization parameters. In no case a global optimal can be guaranteed.
8. The spatial and temporal distributions of optimal pumping are

very much dependent on the specified boundary conditions, initial conditions, aquifer parameter estimates, natural and man-made processes affecting the system, and imposed physical, managerial, operational and other constraints.

9. The proposed model can be easily extended to a multiobjective model to incorporate multiple objectives.

10. The exterior penalty function method together with the embedding approach can be a powerful tool for large scale management of groundwater resources.

11. The applicability of the developed methodologies to solve a problem of large dimensionality will depend on the computing power available. However, computational difficulties such as scaling, sparse matrices and infeasibility of the solutions are not encountered frequently.

12. Simple modifications of the models are required to incorporate various objective functions, other constraints and other complex boundary conditions suitable for different real-life situations.

9.3 SCOPE FOR FUTURE WORK

The following topics are recommended for future studies:

1. Some generic aspects such as uncertainties associated with modeling approximations and parameter estimation, and risks associated with pollutant release may be incorporated explicitly inside the optimization model. Chance constrained

programming or other variations of stochastic optimization may be utilized for this purpose.

2. Application of other nonlinear optimization techniques, particularly genetic algorithms may be explored in terms of their suitability and efficiency in locating a global optimal solution.

3. Other modifications of the proposed models to include various other types of constraints and objectives can be considered.

4. Further studies should be carried out to incorporate more complex transport processes associated with nonlinear degradable pollutants, adsorbent pollutants following nonlinear isotherms, and chemically reactive pollutants.

5. The developed model can be extended to deal with unsaturated flow.

6. The application of the model can be illustrated for the explicit consideration of the conjunctive use of surface water and groundwater.

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APPENDIX

Salient features of NLOGM

```
MAIN ------>VELO1
           (more than one times)

           DIR ------>  VELO1
           (more than one times)

           DISP1 ------->  VELO1
           (more than one times)
                                              |--> HJ -> COF--> DIMN -> VELO1
           DIMN  ------->  VELO1              |          (more
           (more than one times)              |          than    DISCH
                                              |          one
           TRAN                               |          times)  GWFE
                                              |
           DISCH                              |                  STE--> STHICK
           (more than one times)              |
                                              |                         DISP2 --> VELO2
           HJ or PCD ------------------------>|
                                              |                         VELO1
           GWFE                               |
                                              |--------> PCD ---> COF
           STE -------->  STHICK
                                                                  ODS ------> RSET
                          DISP2 ------> VELO2                     (more than  (more
                                                                   one times)  than
                          VELO1                                                one
                                                                  SOVITOS      times)
                                                                  (more than
                                                                   one times)  COF
                                                                               (more
                                                                               than
                                                                               one
                                                                               times)

                                                                               LEAST
```

(a) Calling Subroutines.

COF	:	Computes value of composite objective function.
DIMN	:	Computes dimensionless numbers Re, Cr, Pe and checks the inequality criteria.
DIR	:	Compute directions of velocities at cell nodes.
DISCH	:	Computes value of real objective function.
DISP1	:	Computes convective dispersion coefficients at cell nodes.
DISP2	:	Computes Dispersion Coefficients at Cell boundaries.
GWFE	:	Simulation equation for groundwater flow equation.
HJ	:	Determines Optimal Solution using HJ method.
LEAST	:	Finds the least functional values and its corresponding generating decision variable.
MAIN PROGRAM	:	Prescribe Initial and Boundary Conditions, Bounds Physical and Managerial Constraints, System parameters, Other input data etc.
	:	Incorporates above information and links the subroutines.
ODS	:	Determines Optimal Solution of one dimensional optimization.
PCD	:	Determines Optimal solution using PCD method.
RSET	:	Resets decision variables to suit SQEM method.
STE	:	Simulation equation for solute transport equation.
STHICK	:	Computes saturated thicknesses of at cell boundaries.
SOVITOS	:	Stores decision variables in terms of stage.
TRAN	:	Computes transmissibility.
VELO1	:	Computes velocities at cell nodes.
VELO2	:	Computes velocities at cell boundaries.

(b) Function of subroutines